

Connecting via Winsock to STN

Welcome to STN International! Enter x:X

LOGINID:SSPTAVXR1614

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS	1		Web Page for STN Seminar Schedule - N. America
NEWS	2	JAN 02	STN pricing information for 2008 now available
NEWS	3	JAN 16	CAS patent coverage enhanced to include exemplified prophetic substances
NEWS	4	JAN 28	USPATFULL, USPAT2, and USPATOLD enhanced with new custom IPC display formats
NEWS	5	JAN 28	MARPAT searching enhanced
NEWS	6	JAN 28	USGENE now provides USPTO sequence data within 3 days of publication
NEWS	7	JAN 28	TOXCENTER enhanced with reloaded MEDLINE segment
NEWS	8	JAN 28	MEDLINE and LMEADLINE reloaded with enhancements
NEWS	9	FEB 08	STN Express, Version 8.3, now available
NEWS	10	FEB 20	PCI now available as a replacement to DPCI
NEWS	11	FEB 25	IFIREF reloaded with enhancements
NEWS	12	FEB 25	IMSPRODUCT reloaded with enhancements
NEWS	13	FEB 29	WPINDEX/WPIDS/WPIX enhanced with ECLA and current U.S. National Patent Classification
NEWS	14	MAR 31	IFICDB, IFIPAT, and IFIUDB enhanced with new custom IPC display formats
NEWS	15	MAR 31	CAS REGISTRY enhanced with additional experimental spectra
NEWS	16	MAR 31	CA/CAPLUS and CASREACT patent number format for U.S. applications updated
NEWS	17	MAR 31	LPCI now available as a replacement to LDPCI
NEWS	18	MAR 31	EMBASE, EMBAL, and LEMBASE reloaded with enhancements
NEWS	19	APR 04	STN AnaVist, Version 1, to be discontinued
NEWS	20	APR 15	WPIDS, WPINDEX, and WPIX enhanced with new predefined hit display formats
NEWS	21	APR 28	EMBASE Controlled Term thesaurus enhanced
NEWS	22	APR 28	IMSRESEARCH reloaded with enhancements
NEWS	23	MAY 30	INPAPAFAMDB now available on STN for patent family searching
NEWS	24	MAY 30	DGENE, PCTGEN, and USGENE enhanced with new homology sequence search option
NEWS	25	JUN 06	EPFULL enhanced with 260,000 English abstracts
NEWS	26	JUN 06	KOREAPAT updated with 41,000 documents
NEWS	27	JUN 13	USPATFULL and USPAT2 updated with 11-character patent numbers for U.S. applications
NEWS	28	JUN 19	CAS REGISTRY includes selected substances from web-based collections
NEWS	29	JUN 25	CA/CAPLUS and USPAT databases updated with IPC reclassification data
NEWS	30	JUN 30	AEROSPACE enhanced with more than 1 million U.S.

NEWS 31 JUN 30 patent records  
 EMBASE, EMBAL, and LEMBASE updated with additional  
 options to display authors and affiliated  
 organizations  
 NEWS 32 JUN 30 STN on the Web enhanced with new STN AnaVist  
 Assistant and BLAST plug-in  
 NEWS 33 JUN 30 STN AnaVist enhanced with database content from EPFULL  
 NEWS EXPRESS JUNE 27 08 CURRENT WINDOWS VERSION IS V8.3,  
 AND CURRENT DISCOVER FILE IS DATED 23 JUNE 2008.  
 NEWS HOURS STN Operating Hours Plus Help Desk Availability  
 NEWS LOGIN Welcome Banner and News Items  
 NEWS IPC8 For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that  
 specific topic.

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 agreement. Please note that this agreement limits use to scientific  
 research. Use for software development or design or implementation  
 of commercial gateways or other similar uses is prohibited and may  
 result in loss of user privileges and other penalties.

\*\*\*\*\* STN Columbus \*\*\*\*\*

FILE 'HOME' ENTERED AT 15:50:43 ON 14 JUL 2008

=>  
 Uploading  
 THIS COMMAND NOT AVAILABLE IN THE CURRENT FILE  
 Do you want to switch to the Registry File?  
 Choice (Y/n):  
 Switching to the Registry File...  
 Some commands only work in certain files. For example, the EXPAND  
 command can only be used to look at the index in a file which has an  
 index. Enter "HELP COMMANDS" at an arrow prompt (=>) for a list of  
 commands which can be used in this file.

=> FILE REGISTRY

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 15:51:30 ON 14 JUL 2008  
 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.  
 PLEASE SEE "HELP USAGETERMS" FOR DETAILS.  
 COPYRIGHT (C) 2008 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file  
 provided by InfoChem.

STRUCTURE FILE UPDATES: 13 JUL 2008 HIGHEST RN 1033821-28-1  
 DICTIONARY FILE UPDATES: 13 JUL 2008 HIGHEST RN 1033821-28-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 9, 2008.

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

Uploading C:\Program Files\STNEXP\Queries\10587189.str



```
chain nodes :
1  2  3  4  9 10 12 13 14 15 16 17 18 19
ring/chain nodes :
5  6  7  8 11
chain bonds :
1-2 1-7 2-3 2-4 3-6 4-5 8-9 9-10 11-12 12-13 13-14 13-15 13-16 15-17
16-18
exact/norm bonds :
1-2 1-7 2-3 2-4 3-6 4-5 8-9 11-12 12-13 13-14 13-15 13-16
exact bonds :
9-10 15-17 16-18
```

```
Connectivity :
2:3 E exact RC ring/chain 13:4 E exact RC ring/chain
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS
18:CLASS 19:CLASS
fragments assigned product role:
containing 11
fragments assigned reactant/reagent role:
containing 1
containing 8
containing 19
node mappings:
9:12 8:11 2:13
```

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

=> file casreact

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.46

0.67

FILE 'CASREACT' ENTERED AT 15:51:48 ON 14 JUL 2008

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

COPYRIGHT (C) 2008 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 12 Jul 2008 VOL 149 ISS 3

New CAS Information Use Policies, enter HELP USAGETERMS for details.

```
*****
*
*   CASREACT now has more than 13.8 million reactions   *
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d l1

L1 HAS NO ANSWERS

L1 STR

\*\*\* STRUCTURE DIAGRAM IS NOT AVAILABLE \*\*\*

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 15:52:12 FILE 'CASREACT'

SCREENING COMPLETE - 821 REACTIONS TO VERIFY FROM

41 DOCUMENTS

100.0% DONE 821 VERIFIED

66 HIT RXNS

6 DOCS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED VERIFICATIONS: 14702 TO 18138

PROJECTED ANSWERS: 6 TO 265

L2 6 SEA SSS SAM L1 ( 66 REACTIONS)

=> d l2

L2 ANSWER 1 OF 6 CASREACT COPYRIGHT 2008 ACS on STN

RX(9) OF 14 - REACTION DIAGRAM NOT AVAILABLE

=> d scan ti hit

INVALID SCAN FIELD FOR FILE 'CASREACT'

One or more of the display fields specified are not valid with DISPLAY SCAN in the current file. Enter HELP DSCAN at the arrow prompt (=>) for the list of fields that may be used when scanning the answers.

```
=> D l1 ibib abs
L1 HAS NO ANSWERS
'IBIB ABS ' IS NOT A VALID STRUCTURE FORMAT KEYWORD
Structure Formats
SIA ----- Structure Image, Attributes, and map table if it contains
              data. (Default)
SIM ----- Structure Image.
SAT ----- Structure Attributes and map table if it contains data.
SCT ----- Structure Connection Table and map table if it contains
              data.
SDA ----- All Structure Data (image, attributes, connection table and
              map table if it contains data).
NOS ----- NO Structure data.
ENTER STRUCTURE FORMAT (SIM), NOS:sim
L1          STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
```

Structure attributes must be viewed using STN Express query preparation.

```
=> d l1 ibib abs hitstr
L1 HAS NO ANSWERS
'IBIB ABS HITSTR ' IS NOT A VALID STRUCTURE FORMAT KEYWORD
Structure Formats
SIA ----- Structure Image, Attributes, and map table if it contains
              data. (Default)
SIM ----- Structure Image.
SAT ----- Structure Attributes and map table if it contains data.
SCT ----- Structure Connection Table and map table if it contains
              data.
SDA ----- All Structure Data (image, attributes, connection table and
              map table if it contains data).
NOS ----- NO Structure data.
ENTER STRUCTURE FORMAT (SIM), NOS:nos
L1          STR
```

```
=> d l1
L1 HAS NO ANSWERS
L1          STR
*** STRUCTURE DIAGRAM IS NOT AVAILABLE ***
```

Structure attributes must be viewed using STN Express query preparation.

```
=> s l1 sss full
FULL SEARCH INITIATED 15:57:19 FILE 'CASREACT'
SCREENING COMPLETE -      7766 REACTIONS TO VERIFY FROM      627 DOCUMENTS

100.0% DONE      7766 VERIFIED      472 HIT RXNS (      5 INCOMP)      45 DOCS
SEARCH TIME: 00.00.03

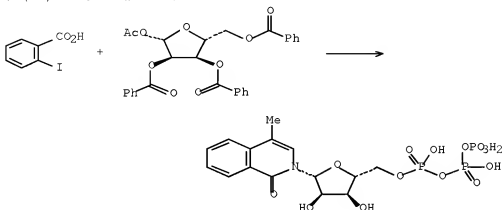
L3              45 SEA SSS FUL L1 (      472 REACTIONS)
```

=> d scan

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Novel nucleotide triphosphates as potent P2Y2 agonists

RX(42) OF 50 - 2 STEPS



NOTE: 2) analogues have similar reaction

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Total Synthesis of Geranylgeranylglycerol Phosphate Enantiomers: Substrates for Characterization of 2,3-O-Digeranylgeranylglycerol Phosphate Synthase

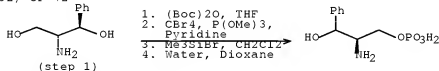
RX(16) OF 33 - REACTION DIAGRAM NOT AVAILABLE

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Synthesis and biological properties of novel sphingosine derivatives

RX(32) OF 72



NOTE: regioselective stage 2

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

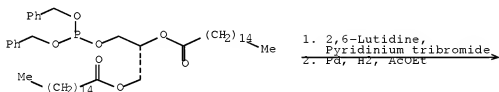
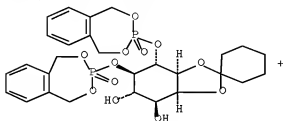
TI NBS-DMSO as a nonaqueous non-basic oxidation reagent for the synthesis of oligonucleotides

RX(33) OF 49 - REACTION DIAGRAM NOT AVAILABLE

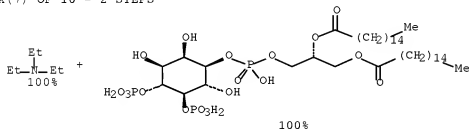
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

TI A short synthesis of dipalmitoylphosphatidylinositol 4,5-bisphosphate via 3-O-selective phosphorylation of a 3,4-free inositol derivative

RX(7) OF 10 - 2 STEPS



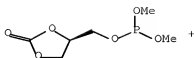
RX(7) OF 10 - 2 STEPS



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

TI Regiospecific Synthesis of 2,6-Di-O-(α-D-mannopyranosyl)phosphatidyl-D-myo-inositol

stereoisomers



1. Pyridinium tribromide,  
Et<sub>3</sub>N, CH<sub>2</sub>Cl<sub>2</sub>
2. Me<sub>3</sub>SiSO<sub>3</sub>CF<sub>3</sub>
3. EtMgCl
4. Pyridine

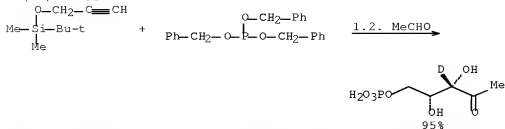
The structure shows a branched polyether chain. At the top, a long alkyl chain  $(CH_2)_{16}Me$  is attached to a carbonyl group, which is linked via an ester bond to a methylene group. This methylene group is part of a chain that includes a phosphonate group  $-O-P(=O)(OH)-O-$ . The phosphonate group is connected to a glycol unit, which is further linked to a complex polyether chain. This chain consists of several sugar-like rings (likely 1,3,5-trisubstituted 1,3,5-hexatrienes) connected by ether linkages. The rings have various hydroxyl ( $OH$ ) groups attached. The entire structure is labeled "stereoisomers" at the bottom.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI The chemical mechanism of D-1-deoxyxylulose-5-phosphate reductoisomerase from *Escherichia coli*

RX(85) OF 110 - 7 STEPS



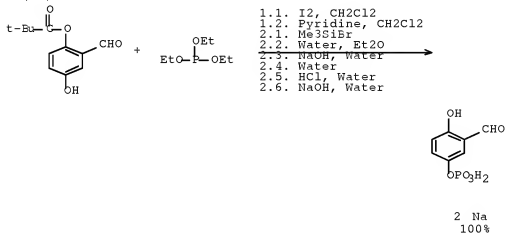
NOTE: 2) in-situ generated reagent (stage 1), regioselective, 4) regioselective, 5) Dess-Martin oxidation, 6) stereoselective

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Cell permeation of a *Trypanosoma brucei* aldolase inhibitor: Evaluation of different enzyme-labile phosphate protecting groups

RX(14) OF 42 - 2 STEPS

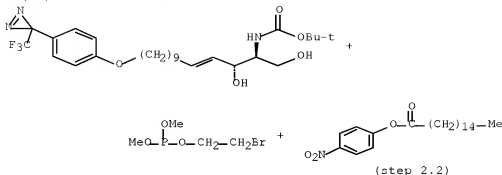


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

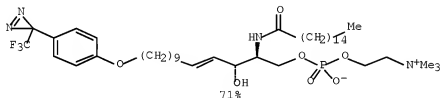
TI Photoaffinity-labeled sphingomyelin analogs and processes thereof

RX(30) OF 53 - 3 STEPS



RX(30) OF 53 - 3 STEPS

- 1.1. CBr4, Pyridine
- 1.2. HCl, Water
- 2.1. F3CCO2H, CH2Cl2
- 2.2. Et3N, THF
3. Me3N, MeOH



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

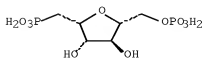
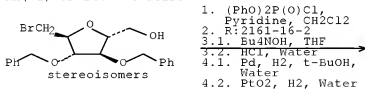
=> d scan 1-45

'1-45' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Synthesis of C-arabinofuranosyl compounds. Phosphonate and carboxylate isosteres of D-arabinose 1,5-bisphosphate

RX(71) OF 140 - 4 STEPS



NOTE: 1) 67% overall, 2) 16 h, 178.degree.

The following are valid formats:

ABS ----- GI and AB  
ALL ----- BIB, AB, IND, RE, Single-step Reactions  
APPS ----- AI, PRAI  
BIB ----- AN, plus Bibliographic Data  
CAN ----- List of CA abstract numbers without answer numbers  
CBIB ----- AN, plus Compressed Bibliographic Data  
DALL ----- ALL, delimited (end of each field identified)  
IABS ----- ABS, indented with text labels  
IALL ----- ALL, indented with text labels  
IBIB ----- BIB, indented with text labels  
IND ----- Indexing data  
IPC ----- International Patent Classifications  
ISTD ----- STD, indented with text labels  
OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels  
  
SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations  
  
MAX ----- Same as ALL  
PATS ----- PI, SO  
SCAN ----- TI and FCRD (random display, no answer number. SCAN  
must be entered on the same line as DISPLAY, e.g.,  
D SCAN.)  
SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for  
all single-step reactions)  
STD ----- BIB, IPC, and NCL  
  
CRD ----- Compact Display of All Hit Reactions  
CRDREF ----- Compact Reaction Display and SO, PY for Reference  
FHIT ----- Reaction Map, Diagram, and Summary for first  
hit reaction  
FHITCBIB --- FHIT, AN plus CBIB  
FCRD ----- First hit in Compact Reaction Display (CRD) format  
FCRDREF ----- First hit in Compact Reaction Display (CRD) format with  
CA reference information (SO, PY). (Default)  
FPATH ----- PATH, plus Reaction Summary for the "long path"  
FSPATH ----- SPATH, plus Reaction Summary for the "short path"  
HIT ----- Reaction Map, Reaction Diagram, and Reaction  
Summary for all hit reactions and fields containing  
hit terms  
OCC ----- All hit fields and the number of occurrences of the  
hit terms in each field. Includes total number of  
HIT, PATH, SPATH reactions. Labels reactions that have  
incomplete verifications.  
PATH ----- Reaction Map and Reaction Diagram for the "long  
path". Displays all hit reactions, except those  
whose steps are totally included within another hit  
reaction which is displayed  
RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)  
RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)  
RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)  
RXS ----- Hit Reaction Summaries (Map and Summary for all hit reactions)  
SPATH ----- Reaction Map and Reaction Diagram for the "short  
path". Displays all single step reactions which  
contain a hit substance. Also displays those

multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

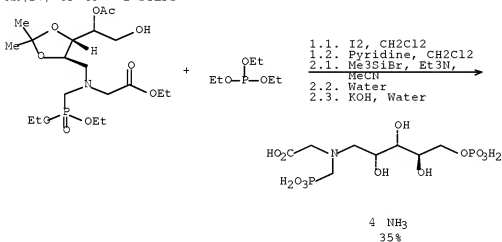
=> d scan 1-45

'1-45' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Synthesis and evaluation of a mechanism-based inhibitor of a 3-deoxy-D-arabino heptulosonate 7-phosphate synthase

RX(17) OF 45 - 2 STEPS



The following are valid formats:

ABS ----- GI and AB  
ALL ----- BIB, AB, IND, RE, Single-step Reactions  
APPS ----- AI, PRAI  
BIB ----- AN, plus Bibliographic Data  
CAN ----- List of CA abstract numbers without answer numbers  
CBIB ----- AN, plus Compressed Bibliographic Data  
DALL ----- ALL, delimited (end of each field identified)  
IABS ----- ABS, indented with text labels  
IALL ----- ALL, indented with text labels  
IBIB ----- BIB, indented with text labels  
IND ----- Indexing data  
IPC ----- International Patent Classifications

ISTD ----- STD, indented with text labels  
 OBIB ----- AN, plus Bibliographic Data (original)  
 OIBIB ----- OBIB, indented with text labels  
  
 SBIB ----- BIB, no citations  
 SIBIB ----- IBIB, no citations  
  
 MAX ----- Same as ALL  
 PATS ----- PI, SO  
 SCAN ----- TI and FCRD (random display, no answer number. SCAN  
                   must be entered on the same line as DISPLAY, e.g.,  
                   D SCAN.)  
 SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for  
                   all single-step reactions)  
 STD ----- BIB, IPC, and NCL  
  
 CRD ----- Compact Display of All Hit Reactions  
 CRDREF ----- Compact Reaction Display and SO, PY for Reference  
 FHIT ----- Reaction Map, Diagram, and Summary for first  
                   hit reaction  
 FHITCBIB --- FHIT, AN plus CBIB  
 FCRD ----- First hit in Compact Reaction Display (CRD) format  
 FCRDREF ----- First hit in Compact Reaction Display (CRD) format with  
                   CA reference information (SO, PY). (Default)  
 FPATH ----- PATH, plus Reaction Summary for the "long path"  
 FSPATH ----- SPATH, plus Reaction Summary for the "short path"  
 HIT ----- Reaction Map, Reaction Diagram, and Reaction  
                   Summary for all hit reactions and fields containing  
                   hit terms  
 OCC ----- All hit fields and the number of occurrences of the  
                   hit terms in each field. Includes total number of  
                   HIT, PATH, SPATH reactions. Labels reactions that have  
                   incomplete verifications.  
 PATH ----- Reaction Map and Reaction Diagram for the "long  
                   path". Displays all hit reactions, except those  
                   whose steps are totally included within another hit  
                   reaction which is displayed  
 RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)  
 RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)  
 RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)  
 RXS ----- Hit Reaction Summaries (Map and Summary for all hit reactions)  
 SPATH ----- Reaction Map and Reaction Diagram for the "short  
                   path". Displays all single step reactions which  
                   contain a hit substance. Also displays those  
                   multistep reactions that have a hit substance in both  
                   the first and last steps of the reaction, except for  
                   those hit reactions whose steps are totally included  
                   within another hit reaction which is displayed

To display a particular field or fields, enter the display field  
 codes. For a list of the display field codes, enter HELP DFIELDS  
 at an arrow prompt (=>). Examples of combinations include: D TI;  
 D BIB RX; D TI, AU, FCRD. The information is displayed in the same order  
 as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH,  
 FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may  
 be used with the DISPLAY command to display the record for a specified  
 Accession Number.

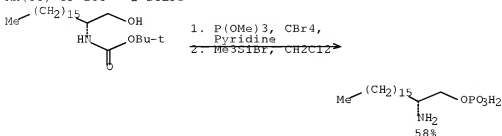
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d scan

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Syntheses of sphingosine-1-phosphate analogues and their interaction with  
EDG/S1P receptors

RX(88) OF 285 - 2 STEPS



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d scan ti hit

INVALID SCAN FIELD FOR FILE 'CASREACT'

One or more of the display fields specified are not valid with DISPLAY  
SCAN in the current file. Enter HELP DSCAN at the arrow prompt (=>)  
for the list of fields that may be used when scanning the answers.

=> d l3 ibib abs hitstr

'HITSTR' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS ----- GI and AB  
ALL ----- BIB, AB, IND, RE, Single-step Reactions  
APPS ----- AI, PRAI  
BIB ----- AN, plus Bibliographic Data  
CAN ----- List of CA abstract numbers without answer numbers  
CBIB ----- AN, plus Compressed Bibliographic Data  
DALL ----- ALL, delimited (end of each field identified)  
IABS ----- ABS, indented with text labels  
IALL ----- ALL, indented with text labels  
IBIB ----- BIB, indented with text labels  
IND ----- Indexing data  
IPC ----- International Patent Classifications  
ISTD ----- STD, indented with text labels  
OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels  
  
SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations  
  
MAX ----- Same as ALL  
PATS ----- PI, SO  
SCAN ----- TI and FCRD (random display, no answer number. SCAN  
must be entered on the same line as DISPLAY, e.g.,  
D SCAN.)  
SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for

all single-step reactions)  
STD ----- BIB, IPC, and NCL

CRD ----- Compact Display of All Hit Reactions  
CRDREF ----- Compact Reaction Display and SO, PY for Reference  
FHIT ----- Reaction Map, Diagram, and Summary for first  
                  hit reaction  
FHITCBIB --- FHIT, AN plus CBIB  
FCRD ----- First hit in Compact Reaction Display (CRD) format  
FCRDREF ---- First hit in Compact Reaction Display (CRD) format with  
                  CA reference information (SO, PY). (Default)  
FPATH ----- PATH, plus Reaction Summary for the "long path"  
FSPATH ----- SPATH, plus Reaction Summary for the "short path"  
HIT ----- Reaction Map, Reaction Diagram, and Reaction  
                  Summary for all hit reactions and fields containing  
                  hit terms  
OCC ----- All hit fields and the number of occurrences of the  
                  hit terms in each field. Includes total number of  
                  HIT, PATH, SPATH reactions. Labels reactions that have  
                  incomplete verifications.  
PATH ----- Reaction Map and Reaction Diagram for the "long  
                  path". Displays all hit reactions, except those  
                  whose steps are totally included within another hit  
                  reaction which is displayed  
RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)  
RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)  
RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)  
RXS ----- Hit Reaction Summaries (Map and Summary for all hit reactions)  
SPATH ----- Reaction Map and Reaction Diagram for the "short  
                  path". Displays all single step reactions which  
                  contain a hit substance. Also displays those  
                  multistep reactions that have a hit substance in both  
                  the first and last steps of the reaction, except for  
                  those hit reactions whose steps are totally included  
                  within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):  
ENTER DISPLAY FORMAT (FCRDREF):o  
'O' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS ----- GI and AB  
ALL ----- BIB, AB, IND, RE, Single-step Reactions  
APPS ----- AI, PRAI  
BIB ----- AN, plus Bibliographic Data  
CAN ----- List of CA abstract numbers without answer numbers  
CBIB ----- AN, plus Compressed Bibliographic Data  
DALL ----- ALL, delimited (end of each field identified)  
IABS ----- ABS, indented with text labels  
IALL ----- ALL, indented with text labels

IBIB ----- BIB, indented with text labels  
 IND ----- Indexing data  
 IPC ----- International Patent Classifications  
 ISTD ----- STD, indented with text labels  
 OBIB ----- AN, plus Bibliographic Data (original)  
 OIBIB ----- OBIB, indented with text labels  
  
 SBIB ----- BIB, no citations  
 SIBIB ----- IBIB, no citations  
  
 MAX ----- Same as ALL  
 PATS ----- PI, SO  
 SCAN ----- TI and FCRD (random display, no answer number. SCAN  
 must be entered on the same line as DISPLAY, e.g.,  
 D SCAN.)  
 SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for  
 all single-step reactions)  
 STD ----- BIB, IPC, and NCL  
  
 CRD ----- Compact Display of All Hit Reactions  
 CRDREF ----- Compact Reaction Display and SO, PY for Reference  
 FHIT ----- Reaction Map, Diagram, and Summary for first  
 hit reaction  
 FHITCBIB --- FHIT, AN plus CBIB  
 FCRD ----- First hit in Compact Reaction Display (CRD) format  
 FCRDREF ---- First hit in Compact Reaction Display (CRD) format with  
 CA reference information (SO, PY). (Default)  
 FPATH ----- PATH, plus Reaction Summary for the "long path"  
 FSPATH ----- SPATH, plus Reaction Summary for the "short path"  
 HIT ----- Reaction Map, Reaction Diagram, and Reaction  
 Summary for all hit reactions and fields containing  
 hit terms  
 OCC ----- All hit fields and the number of occurrences of the  
 hit terms in each field. Includes total number of  
 HIT, PATH, SPATH reactions. Labels reactions that have  
 incomplete verifications.  
 PATH ----- Reaction Map and Reaction Diagram for the "long  
 path". Displays all hit reactions, except those  
 whose steps are totally included within another hit  
 reaction which is displayed  
 RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)  
 RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)  
 RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)  
 RXS ----- Hit Reaction Summaries (Map and Summary for all hit reactions)  
 SPATH ----- Reaction Map and Reaction Diagram for the "short  
 path". Displays all single step reactions which  
 contain a hit substance. Also displays those  
 multistep reactions that have a hit substance in both  
 the first and last steps of the reaction, except for  
 those hit reactions whose steps are totally included  
 within another hit reaction which is displayed

To display a particular field or fields, enter the display field  
 codes. For a list of the display field codes, enter HELP DFIELDS  
 at an arrow prompt (=>). Examples of combinations include: D TI;  
 D BIB RX; D TI, AU, FCRD. The information is displayed in the same order  
 as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH,  
 FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may  
 be used with the DISPLAY command to display the record for a specified  
 Accession Number.

ENTER DISPLAY FORMAT (FCRDFEF):fcrdfef  
'FCRDFEF' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

The following are valid formats:

ABS ----- GI and AB  
ALL ----- BIB, AB, IND, RE, Single-step Reactions  
APPS ----- AI, PRAI  
BIB ----- AN, plus Bibliographic Data  
CAN ----- List of CA abstract numbers without answer numbers  
CBIB ----- AN, plus Compressed Bibliographic Data  
DALL ----- ALL, delimited (end of each field identified)  
IABS ----- ABS, indented with text labels  
IALL ----- ALL, indented with text labels  
IBIB ----- BIB, indented with text labels  
IND ----- Indexing data  
IPC ----- International Patent Classifications  
ISTD ----- STD, indented with text labels  
OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels  
  
SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations  
  
MAX ----- Same as ALL  
PATS ----- PI, SO  
SCAN ----- TI and FCRD (random display, no answer number. SCAN  
must be entered on the same line as DISPLAY, e.g.,  
D SCAN.)  
SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for  
all single-step reactions)  
STD ----- BIB, IPC, and NCL  
  
CRD ----- Compact Display of All Hit Reactions  
CRDREF ----- Compact Reaction Display and SO, PY for Reference  
FHIT ----- Reaction Map, Diagram, and Summary for first  
hit reaction  
FHITCBIB --- FHIT, AN plus CBIB  
FCRD ----- First hit in Compact Reaction Display (CRD) format  
FCRDFEF ----- First hit in Compact Reaction Display (CRD) format with  
CA reference information (SO, PY). (Default)  
FPATH ----- PATH, plus Reaction Summary for the "long path"  
FSPATH ----- SPATH, plus Reaction Summary for the "short path"  
HIT ----- Reaction Map, Reaction Diagram, and Reaction  
Summary for all hit reactions and fields containing  
hit terms  
OCC ----- All hit fields and the number of occurrences of the  
hit terms in each field. Includes total number of  
HIT, PATH, SPATH reactions. Labels reactions that have  
incomplete verifications.  
PATH ----- Reaction Map and Reaction Diagram for the "long  
path". Displays all hit reactions, except those  
whose steps are totally included within another hit  
reaction which is displayed  
RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)  
RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)  
RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)  
RXS ----- Hit Reaction Summaries (Map and Summary for all hit reactions)  
SPATH ----- Reaction Map and Reaction Diagram for the "short

path". Displays all single step reactions which contain a hit substance. Also displays those multistep reactions that have a hit substance in both the first and last steps of the reaction, except for those hit reactions whose steps are totally included within another hit reaction which is displayed

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELD5 at an arrow prompt (=>). Examples of combinations include: D TI; D BIB RX; D TI, AU, FCRD. The information is displayed in the same order as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH, FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may be used with the DISPLAY command to display the record for a specified Accession Number.

ENTER DISPLAY FORMAT (FCRDREF):ti

L3 ANSWER 1 OF 45 CASREACT COPYRIGHT 2008 ACS on STN  
TI Methods for synthesis of carotenoids, including analogs, derivatives, and synthetic and biological intermediates

=> d l3 bib rx

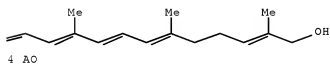
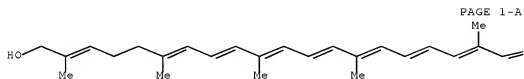
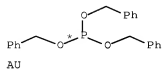
L3 ANSWER 1 OF 45 CASREACT COPYRIGHT 2008 ACS on STN  
AN 148:79206 CASREACT Full-text  
TI Methods for synthesis of carotenoids, including analogs, derivatives, and synthetic and biological intermediates  
IN Lockwood, Samuel F.; Tang, Peng Cho; Nadolski, Geoff; Jackson, Henry L.; Fang, Zhigang; Du, Yishu; Yang, Min; Geiss, William; Williams, Richard; Burdick, David; Braun, Christi L.  
PA Cardax Pharmaceuticals, Inc., USA  
SO PCT Int. Appl., 84pp.  
CODEN: PIXXD2  
DT Patent  
LA English  
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2007147163	A2	20071221	WO 2007-US71482	20070618
	WO 2007147163	A3	20080320		
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW			
	RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA			

PRAI US 2006-814269P 20060616  
OS MARPAT 148:79206

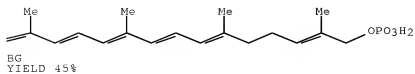
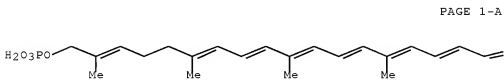
VERIFICATION INCOMPLETE - REACTION MAP DATA UNAVAILABLE

RX(127) OF 304 COMPOSED OF RX(18), RX(19), RX(20)  
 RX(127) AU + 4 AO ==> EG + BH

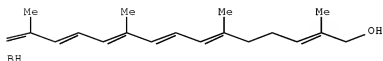
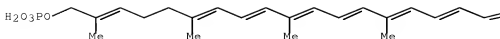


PAGE 1-B

3  
 STEPS  
 →



PAGE 1-B



RX(18) RCT AU 15205-57-9

## STAGE(1)

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON room temperature -> 0 deg C

## STAGE(2)

RGT AZ 7553-56-2 I2

CON SUBSTAGE(1) 10 minutes, 0 deg C

SUBSTAGE(2) 0 deg C -> room temperature

SUBSTAGE(3) 10 minutes, room temperature

PRO AY 877774-61-3

RX(19) RCT AO 19891-75-9

## STAGE(1)

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON room temperature -> 0 deg C

## STAGE(2)

RGT BE 110-86-1 Pyridine

CON 0 deg C

## STAGE(3)

RCT AY 877774-61-3

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON 1 hour, 0 deg C

## STAGE(4)

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON 0 deg C

## STAGE(5)

RGT BF 7647-14-5 NaCl

SOL 7732-18-5 Water

CON 0 deg C

PRO BA 882491-48-7, BB 914359-41-4, BC 882491-49-8D, BD 914359-40-3  
NTE last stage quench

RX(20) RCT BA 882491-48-7, BB 914359-41-4, BC 882491-49-8D, BD 914359-40-3

STAGE(1)

SOL 75-09-2 CH2Cl2

CON room temperature -> 0 deg C

STAGE(2)

RGT BI 10416-59-8 Me3SiN:CMeOSiMe3

CON 0 deg C

STAGE(3)

RGT BJ 2857-57-8 Me3SiBr

CON 15 minutes, 0 deg C

STAGE(4)

RGT AW 121-44-8 Et3N

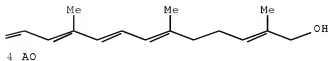
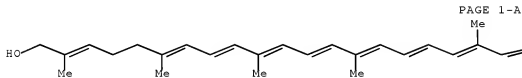
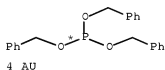
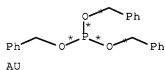
CON 5 minutes, 0 deg C

PRO BG 882491-49-8, BH 914092-96-9

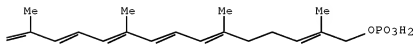
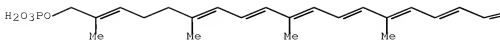
NTE fourth stage quench

RX(128) OF 304 COMPOSED OF RX(18), RX(19), RX(21)

RX(128) 5 AO + 4 AO ==> BK



3  
STEPS  
→



BK

RX(18) RCT AU 15205-57-9

## STAGE(1)

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON room temperature -&gt; 0 deg C

## STAGE(2)

RGT AZ 7553-56-2 I2

CON SUBSTAGE(1) 10 minutes, 0 deg C

SUBSTAGE(2) 0 deg C -&gt; room temperature

SUBSTAGE(3) 10 minutes, room temperature

PRO AY 877774-61-3

RX(19) RCT AO 19891-75-9

## STAGE(1)

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON room temperature -&gt; 0 deg C

## STAGE(2)

RGT BE 110-86-1 Pyridine

CON 0 deg C

## STAGE(3)

RCT AY 877774-61-3

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON 1 hour, 0 deg C

## STAGE(4)

SOL 75-09-2 CH<sub>2</sub>Cl<sub>2</sub>

CON 0 deg C

## STAGE(5)

RGT BF 7647-14-5 NaCl

SOL 7732-18-5 Water  
CON 0 deg C

PRO BA 882491-48-7, BB 914359-41-4, BC 882491-49-8D, BD 914359-40-3  
NTE last stage quench

RX(21) RCT BA 882491-48-7

STAGE(1)  
RGT BB 914359-41-4  $\psi,\psi$ -Carotene-16,16'-diol,  
16-(dihydrogen phosphate) 16'-(phenylmethyl hydrogen  
phosphate), (1E,1'E)-, BC 882491-49-8D  $\psi,\psi$ -Carotene-  
16,16'-diol, 16,16'-bis(dihydrogen phosphate), (1E,1'E)-,  
BD 914359-40-3  $\psi,\psi$ -Carotene-16,16'-diol,  
16-[bis(phenylmethyl) phosphate] 16'-(phenylmethyl hydrogen  
phosphate), (1E,1'E)-  
SOL 75-09-2 CH2Cl2  
CON room temperature -> 0 deg C

STAGE(2)  
RGT BI 10416-59-8 Me3SiN:CMeOSiMe3  
CON 0 deg C

STAGE(3)  
RGT BJ 2857-97-3 Me3SiBr  
CON 15 minutes, 0 deg C

STAGE(4)  
RGT AW 121-44-8 Et3N  
CON 5 minutes, 0 deg C

STAGE(5)  
SOL 67-56-1 MeOH  
CON 0 deg C

STAGE(6)  
RGT Q 124-41-4 NaOMe  
SOL 67-56-1 MeOH  
CON SUBSTAGE(1) 0 deg C  
SUBSTAGE(2) 0 deg C -> room temperature  
SUBSTAGE(3) overnight, room temperature  
SUBSTAGE(4) room temperature -> 0 deg C

STAGE(7)  
SOL 7732-18-5 Water  
CON 5 minutes, 0 deg C

PRO BK 960203-78-5  
NTE fourth stage quench

=> d scan ti

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN  
TI Synthesis of (R)-2-methyl-4-deoxy and (R)-2-methyl-4,5-dideoxy analogues  
of 6-phosphogluconate as potential inhibitors of 6-phosphogluconate

dehydrogenase

HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

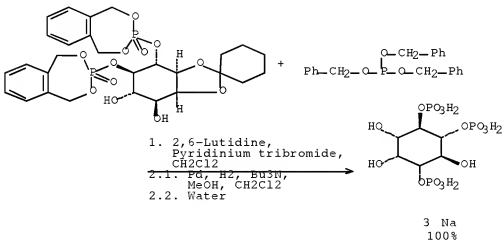
=> d scan ti rxn

'RXN' IS NOT A VALID FORMAT FOR FILE 'CASREACT'

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Regioselective phosphorylation of vicinal 3,4-hydroxy myo-inositol derivative promoted practical synthesis of d-PtdIns(4,5)P2 and D-Ins(1,4,5)P3

RX(21) OF 26 - 2 STEPS



NOTE: 1) regioselective, 2) Na+ and H+cation resin used in last stage

The following are valid formats:

ABS ----- GI and AB  
ALL ----- BIB, AB, IND, RE, Single-step Reactions  
APPS ----- AI, PRAI  
BIB ----- AN, plus Bibliographic Data  
CAN ----- List of CA abstract numbers without answer numbers  
CBIB ----- AN, plus Compressed Bibliographic Data  
DALL ----- ALL, delimited (end of each field identified)  
IABS ----- ABS, indented with text labels  
IALL ----- ALL, indented with text labels  
IBIB ----- BIB, indented with text labels  
IND ----- Indexing data  
IPC ----- International Patent Classifications  
ISTD ----- STD, indented with text labels  
OBIB ----- AN, plus Bibliographic Data (original)  
OIBIB ----- OBIB, indented with text labels  
  
SBIB ----- BIB, no citations  
SIBIB ----- IBIB, no citations  
  
MAX ----- Same as ALL  
PATS ----- PI, SO  
SCAN ----- TI and FCRD (random display, no answer number. SCAN

must be entered on the same line as DISPLAY, e.g.,  
D SCAN.)

SSRX ----- Single-Step Reactions (Map, Diagram, and Summary for  
all single-step reactions)

STD ----- BIB, IPC, and NCL

CRD ----- Compact Display of All Hit Reactions

CRDREF ----- Compact Reaction Display and SO, PY for Reference

FHIT ----- Reaction Map, Diagram, and Summary for first  
hit reaction

FHITCBIB --- FHIT, AN plus CBIB

FCRD ----- First hit in Compact Reaction Display (CRD) format

FCRDREF ----- First hit in Compact Reaction Display (CRD) format with  
CA reference information (SO, PY). (Default)

FPATH ----- PATH, plus Reaction Summary for the "long path"

FSPATH ----- SPATH, plus Reaction Summary for the "short path"

HIT ----- Reaction Map, Reaction Diagram, and Reaction  
Summary for all hit reactions and fields containing  
hit terms

OCC ----- All hit fields and the number of occurrences of the  
hit terms in each field. Includes total number of  
HIT, PATH, SPATH reactions. Labels reactions that have  
incomplete verifications.

PATH ----- Reaction Map and Reaction Diagram for the "long  
path". Displays all hit reactions, except those  
whose steps are totally included within another hit  
reaction which is displayed

RX ----- Hit Reactions (Map, Diagram, Summary for all hit reactions)

RXG ----- Hit Reaction Graphics (Map and Diagram for all hit reactions)

RXL ----- Hit Reaction Long (Map, Diagram, Summary for all hit reactions)

RXS ----- Hit Reaction Summaries (Map and Summary for all hit reactions)

SPATH ----- Reaction Map and Reaction Diagram for the "short  
path". Displays all single step reactions which  
contain a hit substance. Also displays those  
multistep reactions that have a hit substance in both  
the first and last steps of the reaction, except for  
those hit reactions whose steps are totally included  
within another hit reaction which is displayed

To display a particular field or fields, enter the display field  
codes. For a list of the display field codes, enter HELP DFIELDS  
at an arrow prompt (=>). Examples of combinations include: D TI;  
D BIB RX; D TI, AU, FCRD. The information is displayed in the same order  
as the specification. All of the formats, except CRD, CRDREF, FHIT, PATH,  
FPATH, SPATH, FSPATH, FCRD, FCRDREF, HIT, RX, RXG, RXS, SCAN, and OCC, may  
be used with the DISPLAY command to display the record for a specified  
Accession Number.

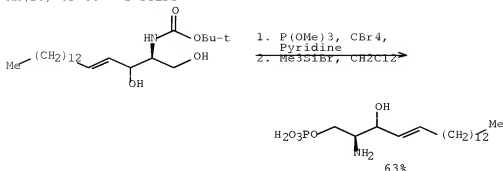
HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d scan

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Syntheses of sphingosine-1-phosphate stereoisomers and analogues and their  
interaction with EDG receptors

RX(18) OF 35 - 2 STEPS

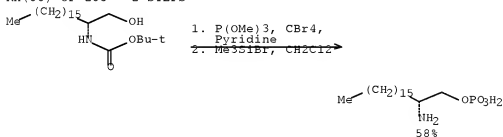


HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):1

L3 45 ANSWERS CASREACT COPYRIGHT 2008 ACS on STN

TI Syntheses of sphingosine-1-phosphate analogues and their interaction with EDG/S1P receptors

RX(88) OF 285 - 2 STEPS



HOW MANY MORE ANSWERS DO YOU WISH TO SCAN? (1):0

=> d scan all

INVALID SCAN FIELD FOR FILE 'CASREACT'

One or more of the display fields specified are not valid with DISPLAY SCAN in the current file. Enter HELP DSCAN at the arrow prompt (=>) for the list of fields that may be used when scanning the answers.

=> d his

(FILE 'HOME' ENTERED AT 15:50:43 ON 14 JUL 2008)

FILE 'REGISTRY' ENTERED AT 15:51:30 ON 14 JUL 2008

L1 STRUCTURE UPLOADED

FILE 'CASREACT' ENTERED AT 15:51:48 ON 14 JUL 2008

L2 6 S L1

L3 45 S L1 SSS FULL

=> d ibib abs fcrd 1-

YOU HAVE REQUESTED DATA FROM 45 ANSWERS - CONTINUE? Y/(N):y

ACCESSION NUMBER: 148:79206 CASREACT Full-text  
 TITLE: Methods for synthesis of carotenoids, including analogs, derivatives, and synthetic and biological intermediates  
 INVENTOR(S): Lockwood, Samuel F.; Tang, Peng Cho; Nadolski, Geoff; Jackson, Henry L.; Fang, Zhiqiang; Du, Yishu; Yang, Min; Geiss, William; Williams, Richard; Burdick, David; Braun, Christi L.  
 PATENT ASSIGNEE(S): Cardax Pharmaceuticals, Inc., USA  
 SOURCE: PCT Int. Appl., 84pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2007147163	A2	20071221	WO 2007-0571482	20070618
WO 2007147163	A3	20080320		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BH, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DO, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, ME, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GO, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA				

PRIORITY APPLN. INFO.: US 2006-814269P 20060616

OTHER SOURCE(S): MARPAT 148:79206

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB A method for synthesizing intermediates for use in the synthesis of carotenoid synthetic intermediates, carotenoid analogs, and/or carotenoid derivs. I [R1, R2 = Ra, Rb, Rc, Rd, Re, Rf; R3 = H, Me; R4 = H, OH, CH2OH, CH2OR5, OR5, wherein at least one R4 = OR5; R5 = alkyl, aryl, alkyl-N(R7)2, aryl-N(R7)2, alkyl-N+(R7)3, aryl-N+(R7)3, alkyl-CO2R7, aryl-CO2R7, alkyl-CO2-, aryl-CO2-, CO2R8, P(=O)(OR8)2, S(=O)(OR8)2, amino acid, peptide, carbohydrate, C(=O)(CH2)nCO2R9, nucleoside, co-antioxidant; R7 = H, alkyl, aryl; R8 = H, alkyl, aryl, CH2Ph, co-antioxidant; R9 = H, alkyl, aryl, P(=O)(OR8)2, S(=O)(OR8)2, amino acid, peptide, carbohydrate, nucleoside, co-antioxidant; n = 1 - 9]. Thus, lycophyll disuccinate disodium salt [II; R' = CH2CH:CHMeCH2OC(=O)(CH2)2CO2Na-(E)] was prepared from crocetinindialdehyde via Wittig reaction with (E,E)-Br-Ph3P+CH2CH:CMcCH2CH2CH:CMcCO2Me in PhMe containing LiOH in MeOH, reduction with Dibal-H/PhMe in THF, diacylation with succinic anhydride in CH2Cl2 containing EtN(CHMe2)2, and sodium salt formation with NaOMe in MeOH. Methods for preparation of crocetinindialdehyde and the phosphonium salt are also given. The carotenoid analog, derivative, or

intermediate may be administered to a subject for the inhibition and/or amelioration of any disease that involves production of reactive oxygen species, reactive nitrogen species, radicals and/or non-radicals. In some embodiments, the invention may include methods for synthesizing chemical compds. including an analog or derivative of a carotenoid. Carotenoid analogs or derivs. may include acyclic end groups. In some embodiments, a carotenoid analog or derivative may include at least one substituent. The substituent may enhance the solubility of the carotenoid analog or derivative such that the carotenoid analog or derivative at least partially dissolves in water.

RX(127) OF 304 - REACTION DIAGRAM NOT AVAILABLE

L3 ANSWER 2 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 147:316938 CASREACT [Full-text](#)

TITLE: The chemical mechanism of D-1-deoxyxylulose-5-phosphate reductoisomerase from Escherichia coli

AUTHOR(S): Wong, Ursula; Cox, Russell J.

CORPORATE SOURCE: School of Chemistry, University of Bristol, Bristol, BS81TS, UK

SOURCE: Angewandte Chemie, International Edition (2007), 46(26), 4926-4929

PUBLISHER: CODEN: ACIEF5; ISSN: 1433-7851

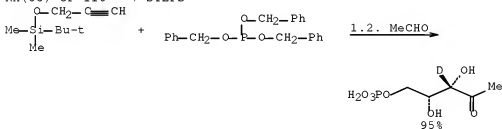
DOCUMENT TYPE: Wiley-VCH Verlag GmbH & Co. KGaA

LANGUAGE: Journal

LANGUAGE: English

AB The 3-[2H]- and 4-[2H]-labeled 1-deoxyxylulose-5-phosphate were synthesized and used to investigate the chemical mechanism of D-1-deoxyxylulose-5-phosphate reductoisomerase (DXR) from E. coli. The observation of inverse secondary kinetic isotope effects for both labeled substrates indicates that DXR uses a retro-aldol/aldol mechanism in which the recombination reaction is the rate-limiting step.

RX(85) OF 110 - 7 STEPS



NOTE: 2) in-situ generated reagent (stage 1), regioselective, 4) regioselective, 5) Dess-Martin oxidation, 6) stereoselective  
 CON: STEP(1.1) room temperature -> -10 deg C; <0 deg C; 10 minutes, <0 deg C; 2 hours, room temperature;  
 room temperature -> -40 deg C  
 STEP(1.2) 1 hour, -40 deg C  
 STEP(1.3) 20 minutes, room temperature  
 STEP(2.1) 30 minutes, reflux; reflux -> 0 deg C  
 STEP(2.2) 0 deg C; 1 hour, 0 deg C; 0 deg C -> room temperature  
 STEP(2.3) room temperature  
 STEP(3) 2 hours, room temperature  
 STEP(4.1) -20 deg C; 20 minutes, -20 deg C -> room temperature  
 STEP(4.2) 40 minutes, -30 deg C; 1 hour, -30 deg C -> room temperature  
 STEP(5.1) 2 hours, room temperature  
 STEP(5.2) 20 minutes, room temperature  
 STEP(5.3) room temperature; room temperature -> -20 deg C  
 STEP(6.1) -20 deg C; 3 hours, -20 deg C -> room temperature  
 STEP(6.3) overnight, room temperature, pH 2  
 STEP(7) 4.5 hours, room temperature, 1 atm

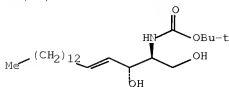
REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

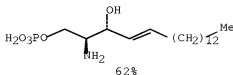
ACCESSION NUMBER: 147:301368 CASREACT [Full-text](#)  
 TITLE: A Concise and Scalable Synthesis of High Enantiopurity (-)-D-erythro-Sphingosine Using Peptidyl Thiol Ester-Boronic Acid Cross-Coupling  
 AUTHOR(S): Yang, Hao; Liebeskind, Lanny S.  
 CORPORATE SOURCE: Department of Chemistry, Emory University, Atlanta, GA, 30322, USA  
 SOURCE: Organic Letters (2007), 9(16), 2993-2995  
 CODEN: ORLEF7; ISSN: 1523-7060  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB A short and efficient synthesis of high enantio-purity (-)-D-erythro-sphingosine has been achieved in 71% yield over 6 steps from N-Boc-L-serine. The key steps are high yield, racemization-free, palladium-catalyzed, copper(I)-mediated coupling of the thio-Ph ester of N-Boc-O-TBS-L-serine with E-1-pentadecenyl boronic acid and the highly diastereoselective reduction of the resulting peptidyl ketone with LiAl(O-t-Bu)3H. By using this concise route (-)-D-erythro-sphingosine can be prepared on large scale and in high enantio- and diastereo-purity (ee >99%, de up to 99%).

RX(60) OF 115 - 2 STEPS



1. P(OEt)<sub>3</sub>, CBr<sub>4</sub>,  
Pyridine  
2.1. Me<sub>3</sub>SiBr, MeCN  
2.2. AcOH  
2.3. Water



62%

CON: STEP(1.1) 0 deg C; 30 minutes, 0 deg C;  
0 deg C -> room temperature; 3 hours, room temperature  
STEP(2.1) 2 hours, room temperature  
STEP(2.2) heated  
STEP(2.3) cooled

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 45 CASREACT COPYRIGHT 2008 ACS on SIN

ACCESSION NUMBER: 146:380213 CASREACT [Full-text](#)

TITLE: A convenient synthesis of 2-C-methyl-D-erythritol 4-phosphate and isotopomers of its precursor

AUTHOR(S): Koumbis, Alexandros E.; Kotoulas, Stefanos S.; Gallos, John K.

CORPORATE SOURCE: Laboratory of Organic Chemistry, Department of Chemistry, Aristotle University of Thessaloniki, Thessaloniki, 541 24, Greece

SOURCE: Tetrahedron (2007), 63(10), 2235-2243

CODEN: TETRAB; ISSN: 0040-4020

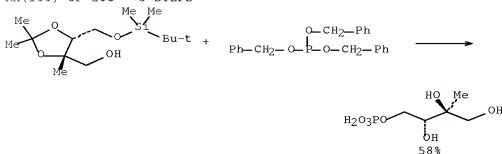
PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new synthetic approach toward 2-C-methyl-D-erythritol 4-phosphate (MEP), a key intermediate in the mevalonate-independent biosynthetic pathway for isoprenoids, and deuterated analogs of its precursor, 2-C-methyl-D-erythritol acetone, is described. This procedure uses 2-C-methyl-D-erythro acetone as starting material and delivers, through a mono-protection strategy, the target compds. in a short way and in high yield.

RX(166) OF 203 - 5 STEPS



CON: STEP(1.1) 1 hour, room temperature  
 STEP(1.2) 24 hours, room temperature  
 STEP(2) 6 hours, room temperature  
 STEP(3.1) room temperature -> -10 deg C; 5 minutes, -10 deg C;  
 1 hour, -10 deg C -> room temperature;  
 room temperature -> 0 deg C  
 STEP(3.2) 30 minutes, 0 deg C  
 STEP(4.1) room temperature -> -10 deg C; 15 minutes, -10 deg C;  
 3 hours, -10 deg C -> room temperature  
 STEP(4.2) room temperature, pH 6  
 STEP(5.1) 25 deg C  
 STEP(5.2) 60 deg C

REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 146:317142 CASREACT [Full-text](#)

TITLE: Novel nucleotide triphosphates as potent P2Y2 agonists

AUTHOR(S): Brookings, Daniel; Davenport, Richard J.; Davis, Jeremy; Galvin, Frances C. A.; Lloyd, Steve; Mack, Stephen R.; Owens, Ray; Sabin, Verity; Wynn, Joanne

CORPORATE SOURCE: Granta Park, UCB-Group, Cambridge, CB1 6GS, UK  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2007), 17(2), 562-565

CODEN: BMCLE8; ISSN: 0960-894X

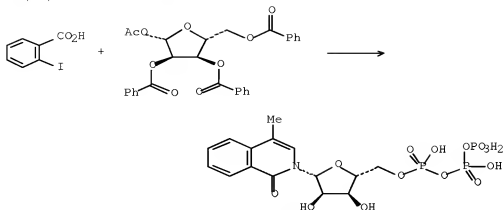
PUBLISHER: Elsevier Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The synthesis and P2Y2 activities of a novel series of nucleoside triphosphates are described. Many of these compds. were potent agonists of the P2Y2 receptor.

RX(42) OF 50 - 2 STEPS



NOTE: 2) analogues have similar reaction

REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 6 OF 45 CASREACT COPYRIGHT 2008 ACS on SIN

ACCESSION NUMBER: 146:100951 CASREACT [Full-text](#)

TITLE: Versatile Synthetic Method for Sphingolipids and Functionalized Sphingosine Derivatives via Olefin Cross Metathesis

AUTHOR(S): Yamamoto, Tetsuya; Hasegawa, Hiroko; Hakogi, Toshikazu; Katsumura, Shigeo

CORPORATE SOURCE: School of Science and Technology, Kwansei Gakuin University, 2-1 Gakuen, Sanda, Hyogo, 669-1337, Japan

SOURCE: Organic Letters (2006), 8(24), 5569-5572

CODEN: ORLEF7; ISSN: 1523-7060

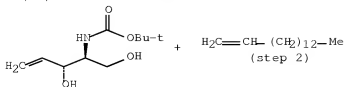
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

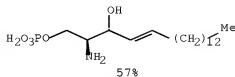
LANGUAGE: English

AB A highly efficient and versatile method for the synthesis of various sphingolipids, such as sphingomyelin, ceramide, sphingosine, sphingosine 1-phosphate, and functionalized sphingosine derivs., was established by two types of combinations of the olefin cross metathesis reaction. One reaction was between the same olefin part and appropriate amino alcs., which were prepared starting from N-Boc-L-serine, and the other was between appropriate olefins and the same amino alc.

RX(74) OF 103 - 3 STEPS



- 1.1. P(OMe)3, CBr4, Pyridine
- 1.2. HCl, Water
2. C-246047-72-3, CH2Cl2
- 3.1. Me3SiBr, CH2Cl2
- 3.2. MeOH



NOTE: 1) molecular sieves used, 2) stereoselective  
 CON: STEP(1.1) -15 deg C; -15 deg C -> room temperature  
 STEP(1.2) 1 deg C  
 STEP(2.1) room temperature; 2 hours, reflux  
 STEP(3.1) 30 minutes, room temperature  
 STEP(3.2) 10 minutes, room temperature

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 7 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 145:489429 CASREACT [Full-text](#)

TITLE: Methods for synthesis of carotenoids, including analogs, derivatives, and synthetic and biological intermediates

INVENTOR(S): Lockwood, Samuel F.; Nadolski, Geoff; Burdick, David; Tang, Peng Cho; Jackson, Henry L.; Fang, Zhiqiang; Du, Yishu; Yang, Min; Geiss, William; Williams, Richard

PATENT ASSIGNEE(S): Hawaii Biotech, Inc., USA

SOURCE: PCT Int. Appl., 59pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006119125	A2	20061109	WO 2006-016487	20060501
WO 2006119125	A3	20070111		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
US 20060293545	A1	20061228	US 2006-415375	20060501
EP 1879902	A2	20080123	EP 2006-751932	20060501
R:	AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,			

IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR  
PRIORITY APPLN. INFO.:

US 2005-67595/P 20050429  
US 2005-691518P 20050617  
US 2005-692682P 20050621  
US 2005-699653P 20050715  
US 2005-702380P 20050726  
US 2005-712350P 20050830  
WO 2006-US16487 20060501

OTHER SOURCE(S): MARPAT 145:489429  
GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB A method for synthesizing intermediates for use in the synthesis of carotenoid synthetic intermediates, carotenoid analogs, and/or carotenoid derivs. I [R1, R2 = Ra, Rb, Rc, Rn, Rm; R3 = H, Me; R4 = H, OH, CH2OH, OR5 with the proviso that at least one R4 = OR5; R5 = alkyl, aryl, alkyl-N(R7)2, aryl-N(R7)2, alkyl-N+(R7)3, aryl-N+(R7)3, alkyl-CO2R7, aryl-CO2R7, alkyl-CO2-, aryl-CO2-, CO2R8, P(:O)(OR8)2, S(:O)(OR8)2, amino acid, peptide, carbohydrate, C(:O)(CH2)nCO2R9, nucleoside, co-antioxidant; R7 = H, alkyl, aryl; R8 = H, alkyl, aryl, CH2Ph, co-antioxidant; R9 = H, alkyl, aryl, P(:O)(OR8)2, S(:O)(OR8)2, amino acid, peptide, carbohydrate, nucleoside, co-antioxidant; n = 1 - 9]. The carotenoid analog, derivative, or intermediate may be administered to a subject for the inhibition and/or amelioration of any disease that involves production of reactive oxygen species, reactive nitrogen species, radicals and/or non-radicals. In some embodiments, the invention may include methods for synthesizing chemical compds. including an analog or derivative of a carotenoid. Carotenoid analogs or derivs. may include acyclic end groups. In some embodiments, a carotenoid analog or derivative may include at least one substituent. The substituent may enhance the solubility of the carotenoid analog or derivative such that the carotenoid analog or derivative at least partially dissolves in water. Thus, lycophyll disuccinate (II) was prepared from acetic acid 3,7-dimethyl-8-oxo-2,6-octadienyl ester via allylic oxidation with NaClO2 in Me3COH containing 2-methyl-2-butene and NaH2PO3, deacetylation with K2CO3 in MeOH, esterification with MeI in aqueous MeOH containing K2CO3, bromination with CBr4 in THF containing PPh3, phosphorylation with PPh3 in EtOAc, Wittig reaction with crocetindialdehyde, all-E-OHC(CMe:CHCH:CH)2CH:CMech:CHCH:CMech CHO, in MeOH containing LiOH, reduction with Dibal-H in THF, and acylation with succinic anhydride in CH2Cl2 containing EtN(CHMe2)2.

RX(78) OF 156 - REACTION DIAGRAM NOT AVAILABLE

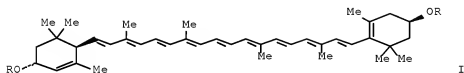
L3 ANSWER 8 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 145:377488 CASREACT [Full-text](#)  
TITLE: Water-dispersible carotenoids, including analogs and derivatives  
INVENTOR(S): Lockwood, Samuel F.; Nadolski, Geoff  
PATENT ASSIGNEE(S): Hawaii Biotech, Inc., USA  
SOURCE: PCT Int. Appl., 77pp.  
CODEN: PIXXD2

DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006102576	A1	20060928	WO 2006-US10726	20060323
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM CA 2611137 A1 20060928 CA 2006-2611137 20060323 US 20070015735 A1 20070118 US 2006-388237 20060323 EP 1877372 A1 20080116 EP 2006-748636 20060323 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR PRIORITY APPLN. INFO.: US 2005-664478P 20050323 WO 2006-US10726 20060323				

OTHER SOURCE(S): MARPAT 145:377488  
 GI



AB Carotenoid analogs or derivs., such as I [R is independently: alkyl; aryl; -alkyl-N(R7)2; -aryl-N(R7)2; -alkyl-N+(R7)3; -aryl-N+(R7)3; -alkyl-CO2R7; -aryl-CO2R7; -alkyl-CO2; -aryl-CO2; -CO2R8; -P(O)(OR8)2; -S(O)(OR8)2; an amino acid; a peptide, a carbohydrate; -C(O)-(CH2)0-CO2R9; a nucleoside residue, or a co-antioxidant; wherein R7 is hydrogen, alkyl, or aryl; wherein R8 is hydrogen, alkyl, aryl, benzyl or a co-antioxidant; wherein R9 is hydrogen; alkyl; aryl; -P(O)(OR8)2; -S(O)(OR8)2; an amino acid; a peptide, a carbohydrate; a nucleoside, or a co-antioxidant], were prepared for therapeutic use in the inhibition and amelioration of diseases resulting in change and/or loss of vision. Thus, lutein disuccinate disodium salt I [R = CO(CH2)2CO2Na] was prepared starting from lutein I (R = H) and succinic anhydride and was evaluated for solubility and antioxidant properties.

RX(9) OF 14 - REACTION DIAGRAM NOT AVAILABLE

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

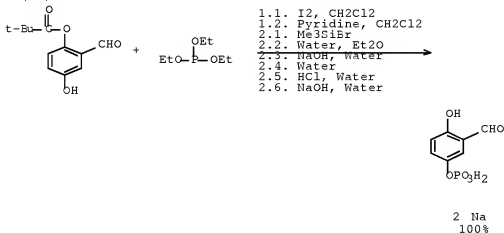
L3 ANSWER 9 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 145:137320 CASREACT [Full-text](#)

TITLE: Cell permeation of a Trypanosoma brucei aldolase inhibitor: Evaluation of different enzyme-labile phosphate protecting groups

AUTHOR(S): Azema, Laurent; Lherbet, Christian; Baudoin, Cecile;  
Blonski, Casimir  
CORPORATE SOURCE: Laboratoire SPCMB, Groupe de Chimie Organique  
Biologique, Universite Paul Sabatier UMR CNRS 5068,  
Toulouse, 31062, Fr.  
SOURCE: Bioorganic & Medicinal Chemistry Letters (2006),  
16(13), 3440-3443  
CODEN: BMCLE8; ISSN: 0960-894X  
PUBLISHER: Elsevier B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB A series of four prodrugs directed against Trypanosoma brucei aldolase bearing various transient enzyme-labile phosphate protecting groups was developed. Herein, we describe the synthesis and evaluation of cell permeation of these prodrugs. The oxymethyl derivative was the most efficient prodrug with a good recovering of the free drug (IC50 = 20 µM) and without any measurable cytotoxicity.

RX(14) OF 42 - 2 STEPS



CON: STEP (1.1) 0 deg C; 0 deg C -> room temperature  
(1.2) 30 minutes, 0 deg C  
(2.1) room temperature  
(2.2) 5 minutes, room temperature  
(2.3) room temperature, neutralized  
(2.4) overnight, room temperature  
(2.5) room temperature, pH 3  
(2.6) room temperature, neutralized

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

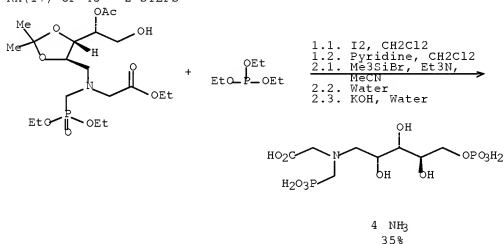
L3 ANSWER 10 OF 45 CASREACT COPYRIGHT 2008 ACS on STN  
ACCESSION NUMBER: 145:83603 CASREACT Full-text  
TITLE: Synthesis and evaluation of a mechanism-based

inhibitor of a 3-deoxy-D-arabino heptulosonate 7-phosphate synthase

AUTHOR(S): Walker, Scott R.; Parker, Emily J.  
CORPORATE SOURCE: Institute of Fundamental Sciences, Massey University,  
Palmerston North, N. Z.  
SOURCE: Bioorganic & Medicinal Chemistry Letters (2006),  
16(11), 2951-2954  
CODEN: BMCLE8; ISSN: 0960-894X  
PUBLISHER: Elsevier B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The first mechanism-based inhibitor of a 3-deoxy-D-arabino heptulosonate 7-phosphate (DAH7P) synthase has been synthesized in 12 steps from D-arabinose, and has been found to be a very slow binding inhibitor of Escherichia coli DAH7P synthase.

RX(17) OF 45 - 2 STEPS



CON: STEP(2.1) 4 deg C  
STEP(2.2) 75 deg C  
STEP(2.3) 75 deg C

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

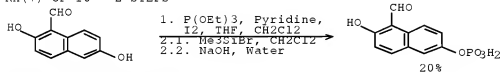
L3 ANSWER 11 OF 45 CASREACT COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 144:365182 CASREACT Full-text  
TITLE: Selective Irreversible Inhibition of Fructose  
1,6-Bisphosphate Aldolase from Trypanosoma brucei  
AUTHOR(S): Dax, Chantal; Duffieux, Francis; Chabot, Nicolas;  
Coincon, Mathieu; Sygusch, Jurgen; Michels, Paul A.  
M.; Blonski, Casimir  
CORPORATE SOURCE: Groupe de Chimie Organique Biologique, LSPCMIB,  
UMR-CNRS 5068, Universite Paul Sabatier, Toulouse,  
31062, Fr.  
SOURCE: Journal of Medicinal Chemistry (2006), 49(5),  
1499-1502  
CODEN: JMCMAR; ISSN: 0022-2623  
PUBLISHER: American Chemical Society  
DOCUMENT TYPE: Journal

LANGUAGE: English

AB An irreversible competitive inhibitor hydroxynaphthaldehyde phosphate was synthesized that is highly selective against the glycolytic enzyme fructose 1,6-bisphosphate aldolase from *Trypanosoma brucei* (causative agent of sleeping sickness). Inhibition involves Schiff base formation by the inhibitor aldehyde with Lys116 followed by reaction of the resultant Schiff base with a second residue. Mol. simulations indicate significantly greater mol. geometries conducive for nucleophilic attack in *T. brucei* aldolase than the mammalian isoenzyme and suggest Ser48 as the Schiff base modifying residue.

RX(7) OF 10 - 2 STEPS



NOTE: 1) regioselective  
CON: STEP(1) 30 minutes, 0 deg C; overnight, room temperature  
STEP(2.1) 3 hours, room temperature  
STEP(2.2) room temperature, pH 7.2

REFERENCE COUNT: 41 THERE ARE 41 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 12 OF 45 CASREACT COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 144:331573 CASREACT [Full-text](#)

TITLE: Total Synthesis of Geranylgeranylglyceryl Phosphate Enantiomers: Substrates for Characterization of 2,3-O-Digeranylgeranylglyceryl Phosphate Synthase

AUTHOR(S): Zhang, Honglu; Shibuya, Kyohei; Hemmi, Hisashi; Nishino, Tokuzo; Prestwich, Glenn D.

CORPORATE SOURCE: Department of Medicinal Chemistry, The University of Utah, Salt Lake City, UT, 84108-1257, USA

SOURCE: Organic Letters (2006), 8(5), 943-946

CODEN: ORLEF7; ISSN: 1523-7060

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

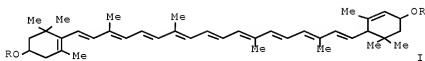
AB To det. the enantioselectivity of (S)-2,3-di-O-geranylgeranylglyceryl phosphate synthase (DGGGPS) from the thermoacidophilic archaeon *Sulfolobus solfataricus*, we developed an efficient enantioselective route to the enantiomeric geranylgeranylglyceryl phosphates (R)-GGGP and (S)-GGGP. Previous routes to these substrates involved enzymic conversions due to the lability of the polyprenyl chains toward common phosphorylation reaction conditions. The synthesis described herein employs a mild tri-Me phosphite/carbon tetrabromide oxidative phosphorylation to circumvent this problem. In contrast to previous results suggesting that only (S)-GGGP can act as the prenyl acceptor substrate, both (R)-GGGP and (S)-GGGP were found to be substrates for DGGGPS.

RX(16) OF 33 - REACTION DIAGRAM NOT AVAILABLE

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 13 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 144:274430 CASREACT [Full-text](#)  
TITLE: The synthesis and aqueous superoxide anion scavenging  
of water-dispersible lutein esters  
AUTHOR(S): Nadolski, Geoff; Cardounel, Arturo J.; Zweier, Jay L.;  
Lockwood, Samuel F.  
CORPORATE SOURCE: Hawaii Biotech, Inc., Aiea, HI, 96701, USA  
SOURCE: Bioorg. Med. Chem. Lett. (2006), 16(4), 775-781  
CODEN: BMCLE8; ISSN: 0960-894X  
PUBLISHER: Elsevier B.V.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI



AB Xanthophyll carotenoids of the C40 series, which includes com. important compds. such as lutein, zeaxanthin, and astaxanthin, have poor aqueous solubility in the native state. Hawaii Biotech, Inc. (HBI) and others have shown that the aqueous dispersibility of derivatized carotenoids can be increased by varying the chemical structure of the esterified moieties. In the current study, the published series of novel, highly water-dispersible C40 carotenoid derivs. has been extended to include derivs. of (3R,3'R,6'R)-lutein [ $\beta,\epsilon$ -carotene-3,3'-diol (I; R = H)]. Two novel derivs. were synthesized by esterification with inorg. phosphate and succinic acid, resp., and subsequently converted to the sodium salts. Red-orange, clear, aqueous suspensions were obtained after addition of these novel derivs. to USP-purified water. Aqueous dispersibility of lutein disuccinate sodium salt (I; R = COCH<sub>2</sub>CH<sub>2</sub>CO<sub>2</sub>Na) was 2.85 mg/mL; the diphosphate salt I [R = P:O(ONa)<sub>2</sub>] demonstrated a >10-fold increase in dispersibility at 29.27 mg/mL. As reported previously, these aqueous suspensions were obtained without the addition of heat, detergents, co-solvents, or other additives. The direct aqueous superoxide scavenging abilities of these novel derivs. were subsequently evaluated by ESR (EPR) spectroscopy in a well-characterized in vitro isolated human neutrophil assay. The novel derivs. were nearly identical aqueous-phase scavengers, demonstrating dose-dependent suppression of the superoxide anion signal (as detected by spin-trap adducts of DEPMPO) in the millimolar range. These lutein-based soft drugs will likely find utility in those com. and clin. applications for which aqueous-phase singlet oxygen quenching and direct radical scavenging may be required.

RX(7) OF 8 - REACTION DIAGRAM NOT AVAILABLE

REFERENCE COUNT: 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

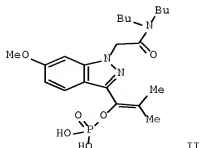
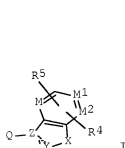
L3 ANSWER 14 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 144:254122 CASREACT [Full-text](#)  
TITLE: Preparation of indazole derivatives and ophthalmic

INVENTOR(S): compositions for treating ocular hypertension  
 Doherty, James B.; Shen, Dong-Ming  
 PATENT ASSIGNEE(S): Merck & Co., Inc., USA  
 SOURCE: PCT Int. Appl., 44 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2006020003	A2	20060223	WO 2005-US25136	20050715
WO 2006020003	A3	20060831		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM AU 2005274972 A1 20060223 AU 2005-274972 20050715 CA 2574078 A1 20060223 CA 2005-2574078 20050715 EP 1771170 A2 20070411 EP 2005-771451 20050715 R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR CN 1988903 A 20070627 CN 2005-80024510 20050715 JP 2008507521 T 20080313 JP 2007-522582 20050715 US 20080032951 A1 20080207 US 2006-630172 20061219 IN 2006CN04793 A 20071005 IN 2006-CN4793 20061229 PRIORITY APPLN. INFO.: US 2004-589444P 20040720 WO 2005-US25136 20050715				

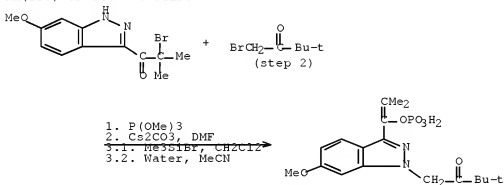
OTHER SOURCE(S): MARPAT 144:254122  
 GI



AB Title compds. I [M, M1, M2 = CH or N; Z = N or C, when Z = N then the bond between Y and Z is a single bond and between X and Y resp. represents CR1=N, CR1=CR1a, CR1a=CR1, or N=CR1, and when Z = C then X = O or S, Y represents CR1 and the bond between Y and Z is a double bond; R4 and R5 independently = H,

OH, alkoxy, etc.; Q = unsatd. phosphonate derivative or substituted carbonyl alkyl derivative; R1 = OH, alkoxy,, unsatd. phosphonate derivative, etc.; R1a = H, (un)substituted alkyl, cycloalkyl, etc.), and their pharmaceutically acceptable salts, are prepared and disclosed as potassium channel blockers suitable for ophthalmic compns. fore treatment of glaucoma and other conditions which leads to elevated intraocular pressure in the eye of a patient. Thus, e.g., I was prepared by amidation of (3-isobutyl-6-methoxy-1H-indazol-1-yl)acetic acid (preparation given) with di-n-butylamine. In assays for evaluating ability to block potassium channels, I was determined to possess IC50's in the range of about 1nM to about 20 µM. This invention also relates to the use of such compds. to provide a neuroprotective effect to the eye of mammalian species, particularly humans.

RX(123) OF 346 - 3 STEPS



NOTE: 1) Perkow reaction, 2) regioselective  
 CON: STEP(1) 21 hours, 62 deg C  
 STEP(2.1) 2 hours, room temperature; 1 day, 50 deg C  
 STEP(3.1) cooled; 2.5 hours, room temperature

L3 ANSWER 15 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:

144:121266 CASREACT [Full-text](#)

TITLE:

NBD-labeled derivatives of the immunomodulatory drug FTY720 as tools for metabolism and mode of action studies

AUTHOR(S):

Ettmayer, Peter; Baumruker, Thomas; Guerini, Danilo; Mechtcheriakova, Diana; Nussbaumer, Peter; Streiff, Markus B.; Billich, Andreas

CORPORATE SOURCE:

Novartis Institutes for BioMedical Research, Vienna, A-1230, Austria

SOURCE:

Bioorganic & Medicinal Chemistry Letters (2006), 16(1), 84-87

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER:

Elsevier B.V.

DOCUMENT TYPE:

Journal

LANGUAGE:

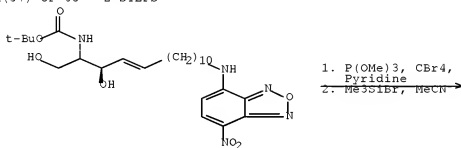
English

AB

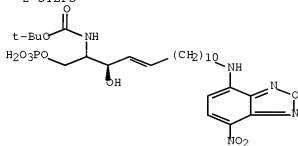
Fluorescently labeled chiral analogs of the immunomodulatory drug FTY720 and its corresponding phosphates with variable aliphatic spacers between the aromatic ring and the NBD label have been synthesized. Determining the influence of the spacer on the in vitro phosphorylation rate by SPHK1 and 2

resulted in the identification of NBD-(R)-AAL 1c,d which are phosphorylated with an efficiency comparable to that of the unlabeled FTY720 analog (R)-AAL. Furthermore, the NBD-(R)-AAL phosphates 10c,d were proven to be a functional S1P receptor agonist.

RX(37) OF 65 - 2 STEPS



RX(37) OF 65 - 2 STEPS



56%

CON: STEP(1) -10 deg C -> room temperature  
STEP(2) room temperature

REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 16 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:

143:229650 CASREACT [Full-text](#)

TITLE:

Photoaffinity-labeled sphingomyelin analogs and processes thereof

INVENTOR(S):

Katsumura, Shigeo; Hakogi, Toshikazu; Shigenari, Toshihiko

PATENT ASSIGNEE(S):

Daiso Co., Ltd., Japan

SOURCE:

U.S. Pat. Appl. Publ., 15 pp.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

1

PATENT INFORMATION:

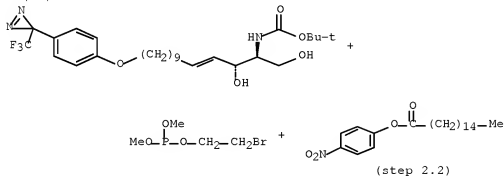
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050182265	A1	20050818	US 2004-934571	20040907
US 7084285	B2	20060801		
JP 2005263774	A	20050929	JP 2004-264995	20040913
PRIORITY APPLN. INFO.:			JP 2004-41750	20040218
OTHER SOURCE(S):	MARPAT 143:229650			

GI

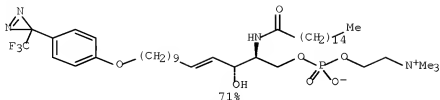
\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB A photoaffinity-labeled sphingomyelin analogs s I (Y1, Y2 are different from each other and are R5 or ZOR1; R5 = C1-20 alkyl, aryl group or C1-6 alkyl group substituted by aryl group, Z is a photoaffinity-labeled group; R1 = C1-20 alkylene) or an optically active compound thereof were prepared Thus, the TFDP-sphingomyelin II was prepared in a multistep procedure starting from the triol III. The TFDP-sphingomyelin IV was similarly prepared

RX(30) OF 53 - 3 STEPS



- 1.1. CBr<sub>4</sub>, Pyridine
- 1.2. HCl, Water
- 2.1. F<sub>3</sub>CCO<sub>2</sub>H, CH<sub>2</sub>Cl<sub>2</sub>
- 2.2. Et<sub>3</sub>N, THF
3. Me<sub>3</sub>N, MeOH



```
CON: STEP(1,1) 0 deg C; 3.5 hours, 0 deg C;
STEP(2,1) C > room temperature
STEP(3,1) room temperature, neutralized
STEP(4,1) 0 deg C; 5 hours, 0 deg C
STEP(5,1) 0 deg C; 1 day, room temperature
STEP(6,1) room temperature; 1 day, room temperature
```

L3 ANSWER 17 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

AUTHOR(S): Dax, Chantal; Coincon, Mathieu; Sygusch, Jurgen;  
Blonski, Casimir

CORPORATE SOURCE: Groupe de Chimie Organique Biologique, LSPCMIB UMR  
CNRS 5068, Université Paul Sabatier, Toulouse, 31062,  
Fr.

SOURCE: Biochemistry (2005), 44(14), 5430-5443  
CODEN: BICHAW; ISSN: 0006-2960

PUBLISHER: American Chemical Society

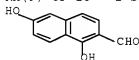
DOCUMENT TYPE: Journal

LANGUAGE: English

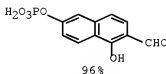
AB Interactions of phosphate derivs. of 2,6-dihydroxynaphthalene (NA-P2) and 1,6-dihydroxy-2-naphthaldehyde (HNA-P, phosphate at position 6) with fructose-1,6-bisphosphate aldolase from rabbit muscle were analyzed by enzyme kinetics, difference spectroscopy, site-directed mutagenesis, mass spectrometry, and mol. dynamics. Enzyme activity was competitively inhibited by NA-P2, whereas HNA-P exhibited slow-binding inhibition with an overall inhibition constant of .apprx.24 nM. HNA-P inactivation was very slowly reversed with t1/2 .apprx.10 days. Mass spectrometry and spectrophotometric absorption indicated that HNA-P inactivation occurs by Schiff base formation. Rates of enzyme inactivation and Schiff base formation by HNA-P were identical and corresponded to .apprx.4 HNA-P mols. bound per aldolase tetramer at maximal inhibition. Site-directed mutagenesis of conserved active site lysine residues 107, 146, and 229 and Asp-33 indicated that Schiff base formation by HNA-P involved Lys-107 and was promoted by Lys-146. Titration of Lys-107 by pyridoxal 5-phosphate yielded a microscopic pKa .apprx.8 for Lys-107, corroborating a role as nucleophile at pH 7.6. Site-directed mutagenesis of Ser-271, an active site residue that binds the Cl-phosphate of dihydroxyacetone phosphate, diminished HNA-P binding and enabled modeling of HNA-P in the active site. Mol. dynamics showed persistent HNA-P phosphate interactions with the Cl-phosphate binding site in the noncovalent adduct. The naphthaldehyde hydroxyl, ortho to the HNA-P aldehyde, was essential for promoting carbinolamine precursor formation by

intramol. catalysis. The simulations indicate a slow rate of enzyme inactivation due to competitive inhibition by the phenate form of HNA-P, infrequent nucleophilic attack in the phenol form, and significant conformational barrier to bond formation as well as electrostatic destabilization of protonated ketimine intermediates. Solvent accessibility by Lys-107 Nz was reduced in the covalent Schiff base complex, and in those instances where water mols. interacted with Lys-107 in the simulations, Schiff base hydrolysis was not mechanistically favorable. The findings at the mol. level corroborate the observed mechanism of slow-binding tight inhibition by HNA-P of muscle aldolase and should serve as a blueprint for future aldolase inhibitor design.

RX(9) OF 15 - 2 STEPS



1.  $P(OEt)_3$ , Pyridine,  
12,  $CH_2Cl_2$   
2.1.  $Me_3SiBF_4$ ,  $CH_2Cl_2$   
2.2. NaOH, Water



CON: STEP(1.1) 1 hour, 0 deg C; 0 deg C -> room temperature  
STEP(2.1) room temperature; 3 hours, room temperature  
STEP(2.2) room temperature, pH 7.5

REFERENCE COUNT: 53 THERE ARE 53 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 18 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 142:392567 CASREACT [Full-text](#)  
TITLE: Synthesis and Evaluation of 1-Deoxy-D-xylulose  
5-Phosphoric Acid Analogues as Alternate Substrates  
for Methylerythritol Phosphate Synthase

AUTHOR(S): Fox, David T.; Poulter, C. Dale  
CORPORATE SOURCE: Department of Chemistry, University of Utah, Salt Lake  
City, UT, 84112, USA

SOURCE: Journal of Organic Chemistry (2005), 70(6), 1978-1985  
CODEN: JOCEAH; ISSN: 0022-3263

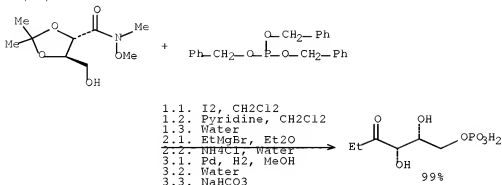
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Four deoxyxylulose phosphate (DXP) analogs were synthesized and evaluated as substrates/inhibitors for methylerythritol phosphate (MEP) synthase. In analogs CF3-DXP (I), CF2-DXP (II), and CF-DXP (III), the three Me hydrogens at C1 of DXP were sequentially replaced by fluorine. In the fourth analog, Et-DXP (IV), the Me group in DXP was replaced by an Et moiety. Analogs I, II, and IV were not substrates for MEP synthase under normal catalytic conditions and were instead modest inhibitors with IC50 values of 2.0, 3.4, and 6.2 mM, resp. In contrast, III was a good substrate ( $k_{cat} = 38 \text{ s}^{-1}$ ,  $K_m = 227 \mu\text{M}$ ) with a turnover rate similar to that of the natural substrate. These results are consistent with a retro-aldol/aldol mechanism rather than an  $\alpha$ -ketol rearrangement for the enzyme-catalyzed conversion of DXP to MEP.

RX(66) OF 78 - 3 STEPS



CON: STEP(1.1) -40 deg C  
STEP(1.2) 10 minutes, -40 deg C; 1 hour,  
STEP(1.3) -40 deg C -> room temperature  
STEP(2.1) room temperature  
STEP(2.2) -40 deg C; 1 hour, -40 deg C  
STEP(3.1) -40 deg C  
STEP(3.2) 6 hours, room temperature  
STEP(3.3) 2 days, room temperature  
STEP(3.3) room temperature, pH 7

REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 19 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 142:374041 CASREACT [Full-text](#)

TITLE: Synthesis and biological properties of novel sphingosine derivatives

AUTHOR(S): Murakami, Teiichi; Furusawa, Kiyotaka; Tamai, Tadakazu; Yoshikai, Kazuyoshi; Nishikawa, Masazumi

CORPORATE SOURCE: National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Ibaraki, 305-8565, Japan

SOURCE: Bioorganic & Medicinal Chemistry Letters (2005), 15(4), 1115-1119  
CODEN: BMCLE8; ISSN: 0960-894X

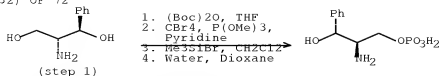
PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Sphingosine-1-phosphate (S-1P) derivs. such as threo-(2S,3S)-analogs, which are C-3 stereoisomers of natural erythro-(2S,3R)-S-1P, have been synthesized starting from -serine or (1S,2S)-2-amino-1-aryl-1,3- propanediols. Threo-(1S,2R)-2-amino-1-aryl-3-bromopropanols (HBr salt) have also been prepared from (1S,2S)-2-amino-1-aryl-1,3-propanediols. The threo-S-1Ps and the threo-amino-bromide derivs. have shown potent inhibitory activity against Ca2+ ion mobilization in HL60 cells induced by erythro-S-1P, suggesting that these compds. would compete with cell surface EDG/S1P receptors.

RX(32) OF 72



NOTE: regioselective stage 2  
 CON: STAGE(2) 5 deg C -> room temperature  
 STAGE(3) 3 hours, room temperature

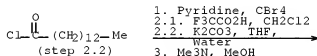
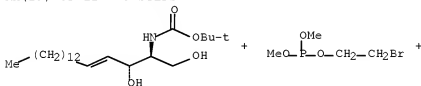
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 20 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

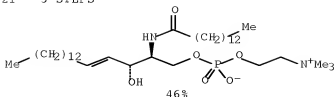
ACCESSION NUMBER: 142:197743 CASREACT Full-text  
 TITLE: Cross metathesis route in sphingomyelin synthesis  
 AUTHOR(S): Hasegawa, Hiroko; Yamamoto, Tetsuya; Hatano, Sho; Hakogi, Toshikazu; Katsumura, Shigeo  
 CORPORATE SOURCE: School of Science and Technology, Kwansei Gakuin University, Hyogo, 669-1337, Japan  
 SOURCE: Chemistry Letters (2004), 33(12), 1592-1593  
 CODEN: CMLTAG; ISSN: 0366-7022  
 PUBLISHER: Chemical Society of Japan  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Cross metathesis reaction of short chain Boc sphingosine using Grubbs' 2nd generation catalyst proceeded in stereoselective manner to afford Boc sphingosine in good yield. An efficient synthesis of sphingomyelin was achieved from the obtained Boc sphingosine using the phosphorylation reagent (MeO)2POCH2CH2Br.

RX(19) OF 21 - 3 STEPS



RX(19) OF 21 - 3 STEPS



CON: STEP(1) 0 deg C  
STEP(2) 0 deg C

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 21 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 142:177000 CASREACT [Full-text](#)

TITLE: A short, concise route to diphosphatidylglycerol (cardiolipin) and its variants

AUTHOR(S): Krishna, U. Murali; Ahmad, Moghis U.; Ali, Shoukath M.; Ahmad, Imran

CORPORATE SOURCE: NeoPharm, Inc., Waukegan, IL, 60085, USA

SOURCE: Lipids (2004), 39(6), 595-600  
CODEN: LPDSAP; ISSN: 0024-4201

PUBLISHER: AOCs Press

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new approach is described for the synthesis of the cardiolipin family of phospholipids that uses phosphonium salt methodol. The method involves the reaction of 2-O-protected glycerol with a trialkyl phosphite derived from 1,2-diacyl-sn-glycerol in the presence of pyridinium bromide perbromide and triethylamine to afford the phosphoric triesters. The synthesis involves three steps and allows the preparation of a wide range of cardiolipins with different substitution patterns and chain lengths, including unsatd. derivs. The use of inexpensive protecting groups and the ease of purification facilitate this synthetic route and allow its scale-up in a higher overall yield (72%) than the literature methods.

RX(11) OF 31 - REACTION DIAGRAM NOT AVAILABLE

REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 22 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 141:424374 CASREACT [Full-text](#)

TITLE: Chemical synthesis of the second messenger nicotinic acid and adenine dinucleoside phosphate by total synthesis of nicotinamide adenine dinucleotide phosphate

AUTHOR(S): Dowden, James; Moreau, Christelle; Brown, Richard S.; Berridge, Georgina; Galione, Antony; Potter, Barry V. L.

CORPORATE SOURCE: Wolfson Laboratory of Medical Chemistry, Department of Pharmacy & Pharmacology, University of Bath, Bath, BA2 7AY, UK

SOURCE: Angewandte Chemie, International Edition (2004), 43(35), 4637-4640

PUBLISHER: CODEN: ACIEF5; ISSN: 1433-7851  
Wiley-VCH Verlag GmbH & Co. KGaA  
DOCUMENT TYPE: Journal  
LANGUAGE: English

AB The first single-isomer synthesis of NADP is reported. Installation and maintenance of sensitive phosphate and pyridinium functionalities were key to success. Significantly, conversion of NADP into the important mammalian second messenger nicotinic acid adenine dinucleotide phosphate (NAADP) was achieved. The *biol.* evaluation of the activity of the release of  $\text{Ca}^{2+}$  ions confirms the identity of NAADP.  $\text{Ca}^{2+}$  release properties against sea-urchin-egg homogenate and spectroscopic characterization are reported.

RX(21) OF 44 - REACTION DIAGRAM NOT AVAILABLE

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 23 OF 45 CASREACT COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 141:390902 CASREACT Full-text

TITLE: Study of 1-Deoxy-D-xylulose-5-phosphate  
Reductoisomerase: Synthesis and Evaluation of  
Fluorinated Substrate Analogues

AUTHOR(S): Wong, Alexander; Munos, Jeffrey W.; Devasthali,  
Vidusha; Johnson, Kenneth A.; Liu, Hung-wen

CORPORATE SOURCE: Division of Medicinal Chemistry, College of Pharmacy  
and Department of Chemistry and Biochemistry,  
University of Texas, Austin, TX, 78712, USA

SOURCE: Organic Letters (2004), 6(20), 3625-3628

CODEN: ORLEF7; ISSN: 1523-7060

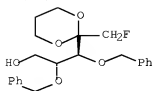
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

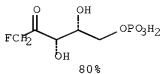
LANGUAGE: English

AB 1-Deoxy-D-xylulose-5-phosphate (DXP) reductoisomerase is a NADPH-dependent enzyme catalyzing the conversion of DXP to methyl-D-erythritol 4-phosphate (MEP). In this study, each of the hydroxyl groups in DXP and one of its C-1 hydrogen atoms, were sep. replaced with a fluorine atom and the effect of the substitution on the catalytic turnover was examined. The 1-fluoro-DXP is a poor substrate, while both 3- and 4-fluoro-DXP behave as noncompetitive inhibitors.

RX(44) OF 237 - 2 STEPS



1. P(OMe)<sub>3</sub>, TeCl<sub>4</sub>,  
2,6-Lutidine,  
CH<sub>2</sub>Cl<sub>2</sub>
- 2.1. Me<sub>3</sub>SiBr, CHCl<sub>3</sub>
- 2.2. Pd, H<sub>2</sub>, water,
- MeOH
- 2.3. HCl, Water
- 2.4. NaHCO<sub>3</sub>



CON: STEP(1) 1.5 hours, room temperature  
STEP(2.1) 1.5 hours, room temperature  
STEP(2.2) 17 hours, room temperature  
STEP(2.3) 12 hours, 37 deg C  
STEP(2.4) room temperature, neutralized

REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 24 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 141:54546 CASREACT Full-text

TITLE: Syntheses of sphingosine-1-phosphate analogues and their interaction with EDG/S1P receptors

AUTHOR(S): Lim, Hyun-Suk; Park, Jeong-Ju; Ko, Kwangseok; Lee, Mee-Hyun; Chung, Sung-Kee

CORPORATE SOURCE: Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea

SOURCE: Bioorganic & Medicinal Chemistry Letters (2004), 14(10), 2499-2503

CODEN: BMCLE8; ISSN: 0960-894X

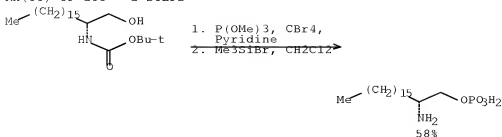
PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Sphingosine-1-phosphate (S1P) is an important regulator of a wide variety of biol. processes acting as an endogenous ligand to EDG/S1P receptors. In an effort to establish structure-activity relationship between EDG/S1P and ligands, the authors report herein homol. modeling study of EDG-1/S1P1, syntheses of S1P analogs, and cell based binding affinity study for EDG/S1P receptors.

RX(88) OF 285 - 2 STEPS



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 25 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 140:321601 CASREACT [Full-text](#)

TITLE: Chemical resolution of 1,2-O-cyclohexylidene-3,4-O-(tetraisopropylidisiloxane-1,3-diyl)-myo-inositol and synthesis of phosphatidyl-D-myo-inositol 3,5-bisphosphate from both L- and D-enantiomers

AUTHOR(S): Han, Fushe; Hayashi, Minoru; Watanabe, Yutaka  
CORPORATE SOURCE: Venture Business Laboratory, Ehime University, Matsuyama, 790-8577, Japan

SOURCE: European Journal of Organic Chemistry (2004), (3), 558-566

CODEN: EJOCFK; ISSN: 1434-193X

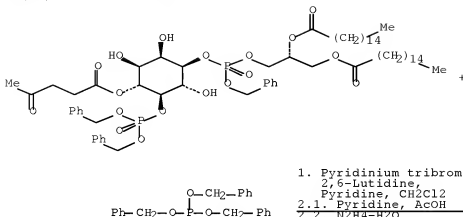
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

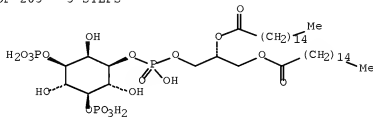
AB Chem. resoln. of a versatile starting material, 1,2-O-cyclohexylidene-3,4-O-(tetraisopropylidisiloxane-1,3-diyl)-myo-inositol, which is used to access naturally occurring inositol phosphates and phosphatidylinositol phosphates, is described. Starting from both D- and L-enantiomers of the material, the synthesis of phosphatidyl-D-myo-inositol 3,5-bisphosphate [PtdIns(3,5)P2] has been conveniently accomplished via convergent routes. One of the key reactions in the synthetic procedure was the regioselective phosphorylation of suitably protected 1,2,4-triol derivs. of inositol. Phosphorylation of the triol attempted in a 1:12 (volume/volume) pyridine/ $\text{CH}_2\text{Cl}_2$  mixture did not proceed at all, whereas in an optimized solvent system, pyridine/ $\text{CH}_2\text{Cl}_2$  (1.1:1, volume/volume), the reaction afforded 68% of the desired 1-O-phosphate as a single product. Further investigation by  $^1\text{H}$  NMR spectroscopy indicated that the reactivity of the three OHs on 1,2,4-triol derivs. is governed by intermol. hydrogen bonding, which may be disrupted by an increase in the proportion of pyridine in the reaction solvent.

RX(80) OF 203 - 3 STEPS



1. Pyridinium tribromide,  
2,6-Lutidine,  
Pyridine, CH<sub>2</sub>Cl<sub>2</sub>  
2.1. Pyridine, AcOH  
2.2. NH<sub>4</sub>-H<sub>2</sub>O  
3. Pd, H<sub>2</sub>, MeOH,  
AcOEt

RX(80) OF 203 - 3 STEPS



CON: STEP(1.1) -42 deg C; 15 minutes, -42 deg C; 2 hours, 0 deg C  
STEP(2.1) 0 deg C  
STEP(2.2) 1.3 hours, 0 deg C -> room temperature  
STEP(3) 16 hours, room temperature, 1 atm

REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 26 OF 45 CASREACT COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 140:5254 CASREACT [Full-text](#)

TITLE: NBS-DMSO as a nonaqueous non-basic oxidation reagent for the synthesis of oligonucleotides

AUTHOR(S): Uzagare, Matthew C.; Padiya, Kamlesh J.; Salunkhe, Manikrao M.; Sanghvi, Yogesh S.

CORPORATE SOURCE: The Institute of Science, Mumbai, 400 032, India

SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(20), 3537-3540

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB A new method for the oxidn. of nucleoside phosphite triester into phosphate triester under non-basic and nonaq. conditions using NBS-DMSO in CH<sub>3</sub>CN has been developed. The utility of this method for solution- and solid-phase synthesis of oligonucleotide is demonstrated.

RX(33) OF 49 - REACTION DIAGRAM NOT AVAILABLE

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 27 OF 45 CASREACT COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 140:5236 CASREACT [Full-text](#)

TITLE: Regioselective phosphorylation of vicinal 3,4-hydroxy myo-inositol derivative promoted practical synthesis of d-PtdIns(4,5)P2 and D-Ins(1,4,5)P3

AUTHOR(S): Han, Fushe; Hayashi, Minoru; Watanabe, Yutaka  
CORPORATE SOURCE: Venture Business Laboratory, Ehime University, Matsuyama, 790-8577, Japan

SOURCE: Tetrahedron (2003), 59(39), 7703-7711

CODEN: TETRA; ISSN: 0040-4020

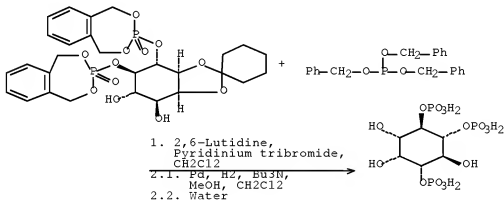
PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The reactivity of 3 and 4-OH in 3,4-diol myo-inositol derivs. were obsd. through the phosphorylation, acylation and silylation. The results indicated that 3-OH is much more reactive than 4-OH, giving regiospecifically 3-mono-functionalized products. This investigation provided a concise methodol. for the synthesis of natural D-form of PtdIns(4,5)P2 and D-Ins(1,4,5)P3 from L-1,2-O-cyclohexylidene-3,4-O-(tetra- iso-Pr disiloxane-1,3-diyl)-myo-inositol.

RX(21) OF 26 - 2 STEPS



3 Na  
100%

NOTE: 1) regioselective, 2) Na+ and H+cation resin used in last stage  
CON: STEP(1.1) -42 deg C; 10 minutes, -42 deg C; 2 hours, 0 deg C  
STEP(2) 3 days, room temperature

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

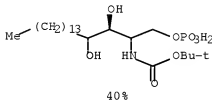
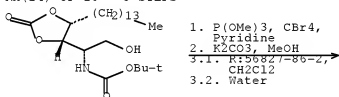
L3 ANSWER 28 OF 45 CASREACT COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 139:101357 CASREACT [Full-text](#)

TITLE: Synthesis of 1-substituted-phytosphingosine: Novel protection of phytosphingosine

AUTHOR(S): Jo, Su Yeon; Kim, Hyoung Cheul; Woo, Seung Woo; Seo, Min Jung; Lee, Ghyeong; Kim, Hyoung Rae  
 CORPORATE SOURCE: Medicinal Science Division, Korea Research Institute of Chemical Technology, Daejeon, 305-600, S. Korea  
 SOURCE: Bulletin of the Korean Chemical Society (2003), 24(3), 267-268  
 CODEN: BKCSDE; ISSN: 0253-2964  
 PUBLISHER: Korean Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 AB Phytosphingosine was protected by the formation of cyclic carbonate in two steps, which could be useful for the derivatizations of 1-position of phytosphingosine. Phytosphingosine-1-phosphate and other derivs. of phytosphingosine were synthesized from the phytosphingosine derivs. protected with cyclic carbonates.

RX(24) OF 26 - 3 STEPS

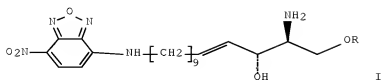


CON: STEP(1) 0 deg C  
 STEP(2) 40 deg C  
 STEP(3.2) 0 deg C

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

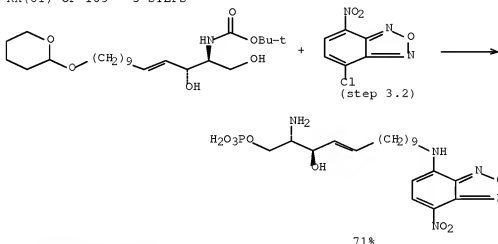
L3 ANSWER 29 OF 45 CASREACT COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 139:52761 CASREACT Full-text  
 TITLE: Synthesis of fluorescence-labeled sphingosine and sphingosine 1-phosphate; effective tools for sphingosine and sphingosine 1-phosphate behavior  
 AUTHOR(S): Hakogi, Toshikazu; Shigenari, Toshihiko; Katsumura, Shigeo; Sano, Takamitsu; Kohno, Takayuki; Igarashi, Yasuyuki  
 CORPORATE SOURCE: School of Science and Technology, Kwansei Gakuin University, Sanda, Hyogo, 669-1337, Japan  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(4), 661-664  
 CODEN: BMCLE8; ISSN: 0960-894X  
 PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB A fluorescence-labeled sphingosine (I; R = H) and sphingosine 1-phosphate (I; R = PO<sub>3</sub>H<sub>2</sub>) have been successfully synthesized from the oxazolidinone Me ester derived from glycidol via monoalkylation and the stereoselective reduction of the resulting ketone. The labeled sphingosine was converted into its phosphate by treatment with sphingosine kinase 1 (SPHK1) from mouse, and in platelets, and it was incorporated into the Chinese Hamster Ovarian (CHO) cells. In addition, MAPK was activated by NBD-Sph-1-P through Edg-1, Sph-1-P receptor.

RX(81) OF 103 - 5 STEPS



CON: STEP(2,2) 50 deg C  
 STEP(3) 60 deg C  
 STEP(4) -10 deg C

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

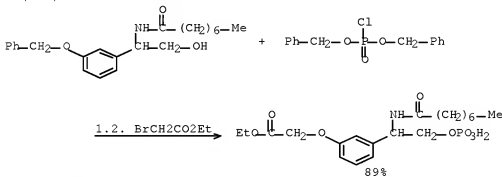
L3 ANSWER 30 OF 45 CASREACT COPYRIGHT 2008 ACS ON STN  
 ACCESSION NUMBER: 139:36724 CASREACT Full-text  
 TITLE: Synthesis of (R)-2-methyl-4-deoxy and  
 (R)-2-methyl-4,5-dideoxy analogues of  
 6-phosphogluconate as potential inhibitors of



Wataru; Ohno, Hiroyuki; Obata, Takaaki; Nakai, Hisao;  
 Toda, Masaaki  
 CORPORATE SOURCE: Fukui Research Institute, Ono Pharmaceutical Co.,  
 Ltd., Sakai, Fukui, 913-8638, Japan  
 SOURCE: Bioorganic & Medicinal Chemistry (2002), 10(12),  
 3757-3786  
 CODEN: BMECEP; ISSN: 0968-0896  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB Discovery of new chem. leads of inhibitors for TNF- $\alpha$  prodn. starting from the chemical modification of 2-(octanoylamino)-2-phenylethyl disodium phosphate (I) is reported. Further biol. studies of I to disclose the site of its action strongly suggested that I inhibits LPS-induced TNF- $\alpha$  expression in the liver and spleen of mice. Structure-activity relationships (SARs) are also discussed and full details including the chemical are reported.

RX(347) OF 529 - 3 STEPS



CON: STEP(1.1) 2 hours, room temperature, 1 atm  
 STEP(1.2) 2 days, room temperature  
 STEP(2.1) 3 hours, room temperature  
 STEP(2.2) 30 minutes, room temperature  
 STEP(3) 20 hours, room temperature, 1 atm

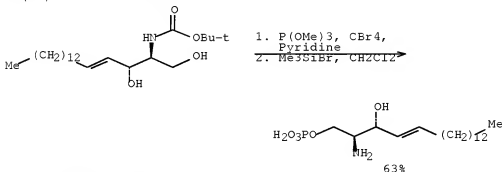
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 32 OF 45 CASREACT COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 138:401994 CASREACT Full-text  
 TITLE: Syntheses of sphingosine-1-phosphate stereoisomers and analogues and their interaction with EDG receptors  
 AUTHOR(S): Lim, Hyun-Suk; Oh, Yong-Seok; Suh, Pann-Ghill; Chung, Sung-Kee  
 CORPORATE SOURCE: Division of Molecular and Life Sciences, Pohang University of Science and Technology, Pohang, 790-784, S. Korea  
 SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(2), 237-240  
 CODEN: BMCLE8; ISSN: 0960-894X  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal

LANGUAGE: English

AB Sphingosine-1-phosphate (S1P) is considered to be an important regulator of diverse biol. processes acting as a natural ligand to EDG receptors. As a preliminary study to develop potent and selective agonist and antagonist for EDG receptors, we report synthesis of S1P stereoisomers and analogs and their binding affinities to EDG-1, -3, and -5.

RX(18) OF 35 - 2 STEPS



CON: STEP(1) 2 hours  
STEP(2) 2 hours

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 33 OF 45 CASREACT COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 138:369095 CASREACT [Full-text](#)

TITLE: A short synthesis of dipalmitoylphosphatidylinositol 4,5-bisphosphate via 3-O-selective phosphorylation of a 3,4-free inositol derivative

AUTHOR(S): Han, Fushe; Hayashi, Minoru; Watanabe, Yutaka  
CORPORATE SOURCE: Venture Business Laboratory, Ehime University, Matsuyama, 790-8577, Japan

SOURCE: Chemistry Letters (2003), 32(1), 46-47  
CODEN: CMLTAG; ISSN: 0366-7022

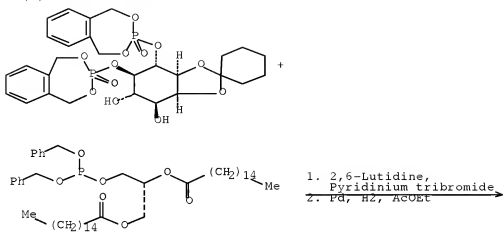
PUBLISHER: Chemical Society of Japan

DOCUMENT TYPE: Journal

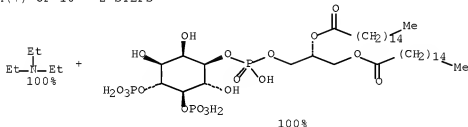
LANGUAGE: English

AB Dipalmitoylphosphatidylinositol 4,5-bisphosphate was conveniently synthesized via the regioselective phosphorylation of L-1,2-O- cyclohexylidene-5,6-di-O-(o-xylylene phosphoryl)-myo-inositol derived from 1,2-O-cyclohexylidene-3,4-O-(tetraoisopropylidisiloxane-1,3-diyl)-myo- inositol.

RX(7) OF 10 - 2 STEPS



RX(7) OF 10 - 2 STEPS



CON: STEP(2) 2 days, room temperature

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 34 OF 45 CASREACT COPYRIGHT 2008 ACS ON STN

ACCESSION NUMBER: 135:284897 CASREACT [Full-text](#)

TITLE: Mechanistic Studies on Thiamin Phosphate Synthase: Evidence for a Dissociative Mechanism

AUTHOR(S): Reddick, Jason J.; Nicewonger, Robb; Begley, Tadgh P.  
CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Cornell University, Ithaca, NY, 14853, USA

SOURCE: Biochemistry (2001), 40(34), 10095-10102  
CODEN: BICHAW; ISSN: 0006-2960

PUBLISHER: American Chemical Society

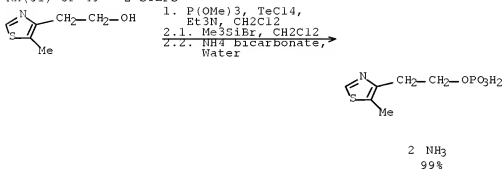
DOCUMENT TYPE: Journal

LANGUAGE: English

AB Thiamin phosphate synthase catalyzes the coupling of 4-methyl-5-( $\beta$ -hydroxyethyl)thiazole phosphate (Thz-P) and 4-amino-5-(hydroxymethyl)-2-methylpyrimidine pyrophosphate (HMP-PP) to give thiamin phosphate. In this paper, we demonstrate that 4-amino-5-(hydroxymethyl)-2-(trifluoromethyl)pyrimidine pyrophosphate (CF<sub>3</sub>-HMP-PP) is a very poor substrate [ $k_{cat}(\text{CH}_3) > 7800k_{cat}(\text{CF}_3)$ ] and that 4-amino-5-(hydroxymethyl)-2-methoxypyrimidine pyrophosphate (CH<sub>3</sub>O-HMP-PP) is a good substrate [ $k_{cat}(\text{OCH}_3) > 2.8k_{cat}(\text{CH}_3)$ ] for the enzyme. We also demonstrate that the enzyme catalyzes positional isotope exchange. These observations are consistent with a

dissociative mechanism (SN1 like) for thiamin phosphate synthase in which the pyrimidine pyrophosphate dissociates to give a reactive pyrimidine intermediate which is then trapped by the thiazole moiety.

RX(31) OF 49 - 2 STEPS



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 35 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 134:86458 CASREACT [Full-text](#)

TITLE: Synthesis of dipalmitoyl-phosphatidylinositol 5-phosphate and its modified biological tools

AUTHOR(S): Watanabe, Yutaka; Ishikawa, Hideki

CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Ehime University, Matsuyama, 790-8577, Japan

SOURCE: Tetrahedron Letters (2000), 41(44), 8509-8512

CODEN: TELEAY; ISSN: 0040-4039

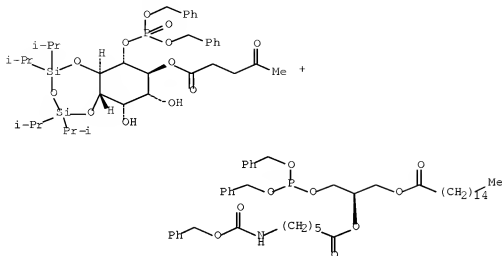
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

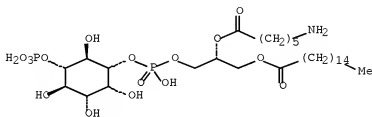
AB Synthesis of a dipalmitoyl analog of phosphatidylinositol 5-phosphate with the racemic inositol skeleton was achieved via a key intermediate, 1,2-cyclohexylidene-3,4-tetraisopropylidisiloxanyl-myo-inositol. Probes bearing a fluorophore, NBD on a fatty acid chain and a resin for affinity chromatog. were also prepared due to biol. interest in cell division.

RX(12) OF 22 - 2 STEPS



RX(12) OF 22 - 2 STEPS

1. Pyridinium tribromide,  
2,6-Lutidine
- 2.1. N<sub>2</sub>H<sub>4</sub>, Pyridine,  
AcOH
- 2.2. Pd, H<sub>2</sub>, t-BuOH,  
Water
- 2.3. Bu<sub>4</sub>N.F, AcOH



NOTE: 1) STEREoselective, 2) STEREoselective

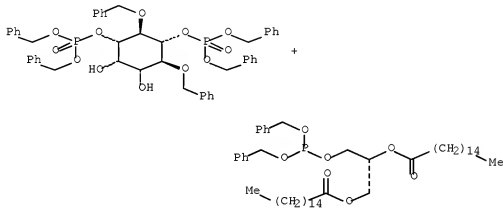
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 36 OF 45 CASREACT COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 133:222919 CASREACT [Full-text](#)  
 TITLE: Concise syntheses of L- $\alpha$ -phosphatidyl-D-myo-inositol 3-phosphate (3-PIP), 5-phosphate (5-PIP), and 3,5-bisphosphate (3,5-PIP<sub>2</sub>)  
 AUTHOR(S): Falck, J. R.; Krishna, U. Murali; Katipally, Kishta Reddy; Capdevila, Jorge H.; Ulug, Emin T.  
 CORPORATE SOURCE: Departments of Biochemistry and Pharmacology, University of Texas Southwestern Medical Center, Dallas, TX, 75390, USA  
 SOURCE: Tetrahedron Letters (2000), 41(22), 4271-4275  
 CODEN: TELEAY; ISSN: 0040-4039  
 PUBLISHER: Elsevier Science Ltd.  
 DOCUMENT TYPE: Journal

LANGUAGE: English

AB Highly efficient, asym. total syntheses of the title phospholipids as well as short-chain and cross-linkable amino ether analogs were achieved in 5-7 steps from a readily available myo-inositol derivative

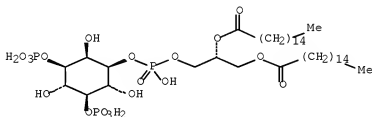
RX(22) OF 88 - 2 STEPS



RX(22) OF 88 - 2 STEPS

1. Pyridinium tribromide,  
CH<sub>2</sub>Cl<sub>2</sub>, Pyridine,  
Et<sub>3</sub>N

2. Pd, H<sub>2</sub>, NaHCO<sub>3</sub>,  
EtOH, Water



79%

NOTE: 1) regioselective

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 37 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

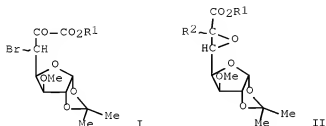
ACCESSION NUMBER: 131:88093 CASREACT Full-text

TITLE: Towards a synthesis of glycidic phosphoenol pyruvic acid derivatives

AUTHOR(S): Coutrot, Philippe; Grison, Claude; Tabyaoui, Mohamed; Tabyaoui, Badia; Dumarcay, Stephane

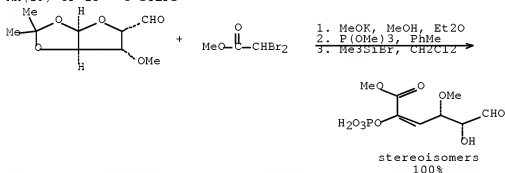
CORPORATE SOURCE: Laboratoire Chimie Organique, Univ. Henri Poincare,

SOURCE: Vandoeuvre-les-Nancy, F-54506, Fr.  
 Synlett (1999), (6), 792-794  
 CODEN: SYNLES; ISSN: 0936-5214  
 PUBLISHER: Georg Thieme Verlag  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI



AB Two synthetic routes are proposed to prep. phospho enol pyruvates of xylose as models of potent phosphoenol pyruvate lyase inhibitors: a Perkow reaction between xylose-derived  $\beta$ -bromo  $\alpha$ -keto esters I ( $R_1 = \text{Me}, \text{CHMe}_2$ ) and  $\text{P(OMe)}_3$ , and a new reaction between xylose-derived  $\alpha$ -bromo glycidates II ( $R_2 = \text{Br}, \text{Cl}$ ;  $R_1 = \text{Me}, \text{CHMe}_2$ ) and  $\text{P(OMe)}_3$ .

RX(19) OF 23 - 3 STEPS



NOTE: 1) STEREOSSELECTIVE, 2) STEREOSSELECTIVE, 3) STEREOSSELECTIVE

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 38 OF 45 CASREACT COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 129:276110 CASREACT Full-text  
 TITLE: Fructose-1,6-bisphosphate aldolase and transketolase: complementary tools for the de novo syntheses of monosaccharides and analogs  
 AUTHOR(S): Andre, C.; Demuyne, C.; Gefflaut, T.; Guerard, C.; Hecquet, L.; Lemaire, M.; Bolte, J.  
 CORPORATE SOURCE: UMR 6504 (SEESIB), Departement de Chimie, Universite Blaise Pascal, Aubiere, 63177, Fr.  
 SOURCE: Journal of Molecular Catalysis B: Enzymatic (1998),

5(1-4), 113-118

CODEN: JMCEF8; ISSN: 1381-1177

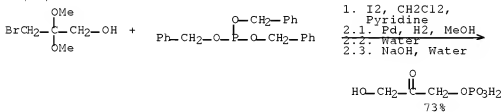
PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This paper reports a new synthesis of bromoacetyl phosphate and dihydroxyacetone phosphate for use in fructose-1,6-bisphosphate aldolase (FB-aldolase) catalyzed syntheses. Then the activities of FB-aldolase and transketolase towards polyhydroxybutanal analogs of erythrose and erythrose-4-phosphate were studied. These activities were high enough to allow the syntheses of rare heptulose-1-phosphates of the d and l series.

RX(16) OF 29 - 2 STEPS



NOTE: 2) 57% yield over five steps from dibromoacetone  
CON: STEP(2.2) 65 deg C

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 39 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 127:162042 CASREACT [Full-text](#)

TITLE: Concise synthesis of L- $\alpha$ -phosphatidyl-D-myo-inositol 3,4-bisphosphate, an intracellular second messenger

AUTHOR(S): Reddy, K. Kishta; Rizo, Josep; Falck, J. R.  
CORPORATE SOURCE: Departments Biochemistry and Pharmacology, University Texas Southwestern Medical Center, Dallas, TX, 75235, USA

SOURCE: Tetrahedron Letters (1997), 38(27), 4729-4730

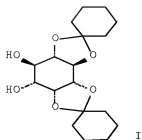
CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

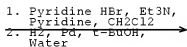
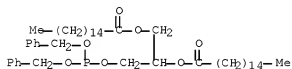
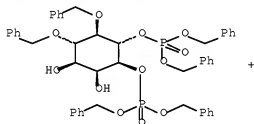
LANGUAGE: English

GI

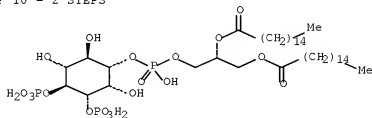


AB A highly efficient, asym. total synthesis of the title phospholipid as well as short chain diester and cross-linkable diether analogs was achieved in six steps from the readily available cyclitol I.

RX (7) OF 10 - 2 STEPS



RX(7) OF 10 - 2 STEPS



5 Na  
96%

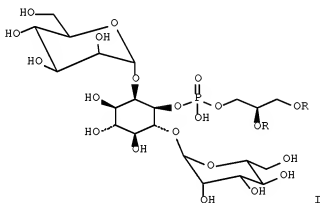
NOTE: 1) key step

REFERENCE COUNT:

16

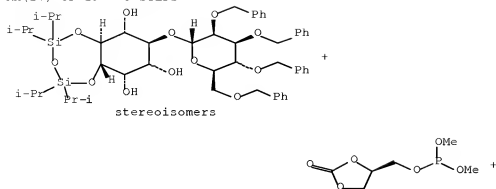
THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 40 OF 45 CASREACT COPYRIGHT 2008 ACS on STN  
 ACCESSION NUMBER: 124:232935 CASREACT [Full-text](#)  
 TITLE: Regiospecific Synthesis of 2,6-Di-O-( $\alpha$ -D-mannopyranosyl)phosphatidyl-D-myo-inositol  
 AUTHOR(S): Watanabe, Yutaka; Yamamoto, Takashi; Ozaki, Shoichiro  
 CORPORATE SOURCE: Faculty of Engineering, Ehime University, Matsuyama, 790, Japan  
 SOURCE: Journal of Organic Chemistry (1996), 61(1), 14-15  
 CODEN: JOCEAH; ISSN: 0022-3263  
 PUBLISHER: American Chemical Society  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 GI

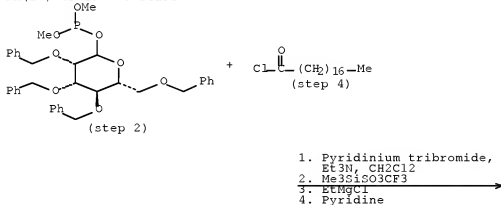


AB A concise synthesis of 2,6-di-O- $\alpha$ -D-mannopyranosylphosphatidyl-D-myo-inositol I [R = CO(CH<sub>2</sub>)<sub>16</sub>Me] has been accomplished by completely regioselective introduction of the requisite substituents on myo-inositol. The pivotal intermediate, 1,2-O-cyclohexylidene-3,4-O-(tetraisopropylidisiloxane-1,3-diyl)-myo-inositol, was glycosylated regioselectively at the 6-position using a mannopyranosyl phosphite as the glycosyl donor. After removing the cyclohexylidene group, the resultant 1,2-diol derivative was phosphorylated by the reaction with a glycerol phosphite in the presence of pyridinium bromide perbromide to afford regioselectively 1-O-phosphate. This was then glycosylated regio- and stereoselectively at the 2-position by the phosphite approach as above. The 1,2-O-carbonyl protecting group in the glycerol moiety was removed by the reaction with the ethylmagnesium chloride without the migration of the phosphite function, and the resulting diol was acylated and finally deprotected.

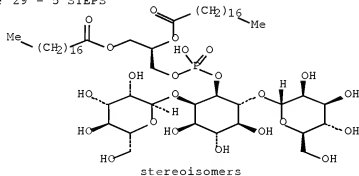
RX (27) OF 29 - 5 STEPS



RX (27) OF 29 - 5 STEPS



RX (27) OF 29 - 5 STEPS



NOTE: 1) 83% overall, regioselective, 4) 73% OVERALL, 5) ISOMERIC  
REACTANTS ALSO PRESENT

TITLE: Synthesis of C-arabinofuranosyl compounds.  
Phosphonate and carboxylate isosteres of D-arabinose 1,5-bisphosphate

AUTHOR(S): Maryanoff, Bruce E.; Nortey, Samuel O.; Inners, Ruth R.; Campbell, Susan A.; Reitz, Allen B.; Liotta, Dennis

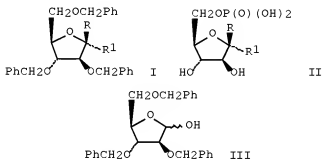
CORPORATE SOURCE: Chem. Res. Dep., McNeil Pharm., Spring House, PA, 19477, USA

SOURCE: Carbohydrate Research (1987), 171, 259-78  
CODEN: CRBRAT; ISSN: 0008-6215

DOCUMENT TYPE: Journal

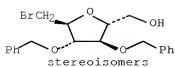
LANGUAGE: English

GI

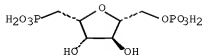


AB Electrophile-mediated cyclization. of 3,4,6-tri-O-benzyl-1,2-dideoxy-D-arabino-hex-1-enitol with N-bromosuccinimide yielded primarily 2,5-anhydro-3,4,6-tri-O-benzyl-1-bromo-1-deoxy-D-glucitol (I;  $\text{R} = \text{CH}_2\text{Br}$ ,  $\text{R}_1 = \text{H}$ ). This apparently kinetically controlled reaction was of key importance in the successful synthesis of a phosphonate analog of  $\beta$ -D-arabinose 1,5-bisphosphate [II;  $\text{R} = \text{OP(O)(OH)}_2$ ,  $\text{R}_1 = \text{H}$ ], namely, 2,5-anhydro-1-deoxy-1-phosphono-D-glucitol 6-phosphate [II;  $\text{R} = \text{CH}_2\text{OP(O)(OH)}_2$ ,  $\text{R}_1 = \text{H}$ ] with high stereoselectivity. By contrast, condensation of the sodium salt of tetra-Et methylenediphosphonate and 2,3,5-tri-O-benzyl-D-arabinose (III) gave a phosphonate compound slightly enriched in the 2,5-anhydro-D-mannitol ( $\alpha$ ) isomer. In the Wittig-Michael reaction of stabilized phosphoranes with (III), the  $\alpha$  isomer preponderated. Since equilibration of Me 3,6-anhydro-4,5,7-tri-O-benzyl-2-deoxy-D-glycero-D-galacto- (I;  $\text{R} = \text{H}$ ,  $\text{R}_1 = \text{CH}_2\text{O}_2\text{Me}$ ) and -D-gulo-heptonate (I;  $\text{R} = \text{CH}_2\text{CO}_2\text{Me}$ ,  $\text{R}_1 = \text{H}$ ) (5:1) resulted in a 1:1  $\alpha$ : $\beta$  ratio, the preference for the 2,5-anhydro-D-mannitol ( $\alpha$ ) isomer probably reflects a kinetic bias. The carbomethoxy anomers were converted independently into the  $\alpha$  and  $\beta$  carboxylate isosteres [II ( $\text{R} = \text{H}$ ,  $\text{R}_1 = \text{CH}_2\text{CO}_2\text{H}$ ;  $\text{R} = \text{CH}_2\text{CO}_2\text{H}$ ,  $\text{R}_1 = \text{H}$ ), resp.] of D-arabinose 1,5-diphosphate. Empirical force field calcs. (MMP2) and NMR expts. were conducted on the pairs of diastereomers I ( $\text{R} = \text{H}$ ,  $\text{R}_1 = \text{CH}_2\text{Br}$ ;  $\text{R} = \text{CH}_2\text{Br}$ ,  $\text{R}_1 = \text{H}$ ; and  $\text{R} = \text{H}$ ,  $\text{R}_1 = \text{CH}_2\text{CO}_2\text{Me}$ ;  $\text{R} = \text{CH}_2\text{CO}_2\text{Me}$ ,  $\text{R}_1 = \text{H}$ ). The calcs. predict that the  $\alpha$  and  $\beta$  anomers of each pair have similar energies, differing by only 2.1 kJ/mol. Compds. II [ $\text{R} = \text{CH}_2\text{P(O)(OH)}_2$ ,  $\text{CH}_2\text{CO}_2\text{H}$ ,  $\text{R}_1 = \text{H}$ ;  $\text{R} = \text{H}$ ,  $\text{R}_1 = \text{CH}_2\text{CO}_2\text{H}$ ] were evaluated for biol. activity.

RX(71) OF 140 - 4 STEPS



1. (PhO)<sub>2</sub>P(O)Cl,  
Pyridine, CH<sub>2</sub>Cl<sub>2</sub>
2. R:2161-16-2
- 3.1. Bu<sub>4</sub>NOH, THF
- 3.2. HCl, Water
- 4.1. Pd, H<sub>2</sub>, t-BuOH,  
Water
- 4.2. PtO<sub>2</sub>, H<sub>2</sub>, Water



NOTE: 1) 67% overall, 2) 16 h, 178.degree.

L3 ANSWER 42 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER:

104:225103 CASREACT [Full-text](#)

TITLE:

Stereoselectivity in the electrophile-promoted cyclizations of a hydroxyolefin derived from arabinose. Synthesis of a phosphonate isostere of β-D-arabinose-1,5-diphosphate

AUTHOR(S):

Reitz, Allen B.; Nortey, Samuel O.; Maryanoff, Bruce E.

CORPORATE SOURCE:

Chem. Res. Dep., McNeil Pharm., Spring House, PA, 19477, USA

SOURCE:

Tetrahedron Letters (1985), 26(33), 3915-18

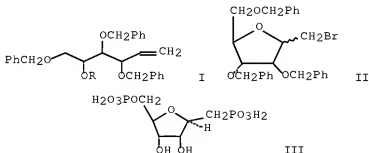
DOCUMENT TYPE:

CODEN: TELEAY; ISSN: 0040-4039

LANGUAGE:

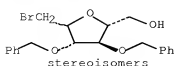
Journal  
English

GI

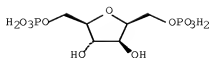


AB Cyclization of hydroxyolefin I [R = H, SiMe<sub>2</sub>CMe<sub>3</sub>, CH<sub>2</sub>O(CH<sub>2</sub>)<sub>2</sub>SiMe<sub>3</sub>] with NBS or Hg(OAc)<sub>2</sub> yielded predominantly the β isomer of a C-arabinofuranoside II. II was acetylated, phosphorylated and hydrolyzed to yield isostere III.

RX(36) OF 50 - 3 STEPS



1. (PhO)2P(O)Cl,  
Pyridine
2. R: 2161-16-2
- 3.1. MeNH<sup>+</sup>OH<sup>-</sup>
- 3.2. Pd, H2
- 3.3. Pt, H2



2 Na

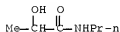
L3 ANSWER 43 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 101:37906 CASREACT [Full-text](#)  
 TITLE: Phosphoenol pyruvamides. Amide-phosphate interactions in analogs of phosphoenol pyruvate  
 AUTHOR(S): Kluger, Ronald; Chow, Jane Frances; Croke, James J.  
 CORPORATE SOURCE: Dep. Chem., Univ. Toronto, Toronto, ON, M5S 1A1, Can.  
 SOURCE: Journal of the American Chemical Society (1984), 106(14), 4017-20  
 CODEN: JACSAT; ISSN: 0002-7863

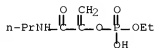
DOCUMENT TYPE: Journal  
 LANGUAGE: English

AB CH2:C[OP(O)(OR)2]CONHR1 (I; R = Et, R1 = Pr, Ph) were obtained in the reaction of (EtO)3P with BrCH2COCONHR1. The 1st order hydrolysis kinetics, of the Et ester portion, of I are 4 orders of magnitude faster than that estimated for (EtO)3P (under comparable conditions) indicating neighboring participation by the carboxamide group. The Et group in I is cleaved much more slowly than that in unconjugated enol phosphate monoesters indicating that the I hydrolysis mechanism involves amide addition to the adjacent phosphate to form a reactive cyclic intermediate. The implication of I hydrolysis for phosphoenol pyruvate studies in enzyme systems and for peptide-nucleotide interactions are discussed.

RX(25) OF 26 - 4 STEPS



1. CrO3
2. Br2
3. P(OEt)3
4. NaI



Na

L3 ANSWER 44 OF 45 CASREACT COPYRIGHT 2008 ACS on STN

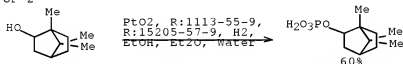
ACCESSION NUMBER: 60:61195 CASREACT [Full-text](#)  
 TITLE: Synthesis of testosterone dimethyl phosphate, bornyl phosphate, and adenosine 5'-phosphate  
 AUTHOR(S): Hata, Tsujiaki; Mukaiyama, Teruaki  
 CORPORATE SOURCE: Tokyo Inst. Technol.

SOURCE: Bulletin of the Chemical Society of Japan (1964),  
37(1), 103-4  
CODEN: BCSJA8; ISSN: 0009-2673  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB (MeO)3P added to a soln. of 1 mole testosterone and 1 mole NCCHBrCONH2 (I) in dry ether at -40° gave 62% testosterone di-Me phosphate (II). Borneol with I and (PhCH2O)3P, followed by hydrogenolysis to remove the benzyl group, gave 60% bornyl phosphate (III). 2',3'-O- Isopropylideneadenosine (1 mole) treated with 1 mole NCCHBrCONH2 and 1 mole (PhCH2O)3P, followed by hydrogenolysis and hydrolysis gave 62% adenosine 5'-phosphate.

RX(1) OF 2

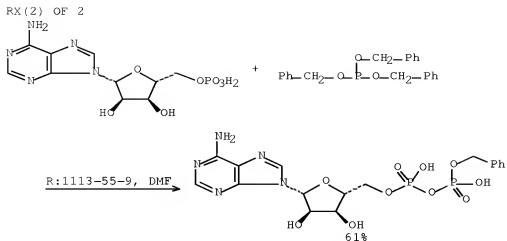


NOTE: Classification: O-Phosphorisation; Hydrogenolysis; Catalysis; Oxidation; # Conditions: H2/NCCHBrCONH2; (PhCH2O)3P; Et2O 20 deg; 2h 20 deg overnight; H2/PtO2 EtOH H2O

L3 ANSWER 45 OF 45 CASREACT COPYRIGHT 2008 ACS ON STN  
ACCESSION NUMBER: 60:15998 CASREACT Full-text  
TITLE: Pyrophosphates  
INVENTOR(S): Mukaiyama, Teruaki; Hata, Tsujiaki  
PATENT ASSIGNEE(S): Asahi Chemical Industry Co., Ltd.  
SOURCE: 3 pp.  
DOCUMENT TYPE: Patent  
LANGUAGE: Unavailable  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 38017308	B4	19630906	JP	19620331
DE 1200819			DE	
FR 1372445			FR	
GB 1007770			GB	
US 3188310		19650608	US 1963-269719	19630401
PRIORITY APPLN. INFO.:			JP	19620331

AB A mixt. of 1.54 g. diethyl phosphite and 1.63 g.  $\alpha$ - monobromocyclohexanecarboxamide in 150 ml. Et2O is kept at -50°, a solution of 1.24 g. trimethyl phosphate in 15 ml. Et2O gradually added, the mixture allowed to stand 2 hrs. and filtered, and the filtrate distilled in vacuo to give 2.4 g. dimethyl diethyl pyrophosphate, b0.004 100-6°. Similarly prepared are tetraethyl pyrophosphate (b1 135-6°), diethyl dibutyl pyrophosphate (b0.02 114-18°), bis(p-nitrophenyl) N-cyclohexylphosphamidate (m. 172-3°), and monobenzyl 5'-adenosine diphosphate.



NOTE: Classification: Phosphorylation; Condensation; # Conditions:  
H2NCOCH(Br)CN; BuNH2, DMF; 6h; 20 deg 24h

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	340.99	341.66
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE	TOTAL
	ENTRY	SESSION
CA SUBSCRIBER PRICE	-33.75	-33.75
STN INTERNATIONAL LOGOFF AT 16:25:52 ON 14 JUL 2008		